

AD 749879

**INFRARED ABSORPTION BANDS
OF NITROUS OXIDE**

by

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Contract No. F19628-69-C-0263
Project No. 5130

Final Report
15 May 1969 - 14 July 1972

Approved for public release; distribution unlimited.

Contract Monitor: Robert A. McClatchey
Optical Physics Laboratory

Sponsored by
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Contractor: Philco-Ford Corporation

Effective Date of Contract - 15 May 1969

Contract No. F19628-69-C-0263

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Contract Expiration Date -
14 July 1972

ACCESSION for	
NTIS	White Section <input checked="" type="checkbox"/>
DDC	Ref. Section <input type="checkbox"/>
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UNCLASSIFIED

Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body or abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) Philco-Ford Corporation Aeronutronic Division Newport Beach, California 92663		2a. REPORT SECURITY CLASSIFICATION Unclassified	
		2b. GROUP	
3. REPORT TITLE INFRARED ABSORPTION BANDS OF NITROUS OXIDE			
4. DESCRIPTIVE NOTES (Type of report and inclusive dates) Scientific Final 15 May 1961 - 14 July 1972 Approved 19 July 1972			
5. AUTHOR(S) (First name, middle initial, last name) Darrell E. Burch David A. Gryvnak John D. Pembroke			
6. REPORT DATE June 1972	7a. TOTAL NO OF PAGES 85	7b. NO OF PAGES 40	
8a. CONTRACT OR GRANT NO F19628-69-C-0263 ARPA Order No. 1366 b. Project, Task, Work Unit Nos. 5130 n/a n/a c. DOD Element 62301D d. DOD Supplement n/a		9a. ORIGINATOR'S REPORT NUMBER(S) U-5037 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report) AFCRL-72-0387	
10. DISTRIBUTION STATEMENT A - Approved for public release; distribution unlimited.			
11. SUPPLEMENTARY NOTES Tech, Other		12. SPONSORING MILITARY ACTIVITY Air Force Cambridge Research Laboratories L. G. Hanscom Field (OP) Bedford, Massachusetts 01730	
13. ABSTRACT All of the infrared absorption bands of N ₂ O that are sufficiently intense to absorb significantly in the earth's atmosphere are summarized. The information required to calculate the positions of most of the absorption lines is tabulated along with the intensities of the band systems. The required data on line positions that are not yet available are pointed out. Spectral plots of transmittance and of the absorption coefficient are included for several bands between 530 and 760/cm ⁻¹ and between 1585 and 4000/cm ⁻¹ .			

1A

DD FORM 1 NOV 65 1473

UNCLASSIFIED

Security Classification

UNCLASSIFIED
Security Classification

14 KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
N_2O Atmospheric Transmission Absorption						

UNCLASSIFIED
Security Classification

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ACKNOWLEDGMENT

The authors wish to acknowledge the major contribution of Professor William S. Benedict of the University of Maryland to the work reported here. He is responsible for the interpretation of many of the data, particularly those dealing with relative intensities. His suggestions and his cooperation have been very helpful and are greatly appreciated.

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SECTION 1

BACKGROUND

INTRODUCTION AND SUMMARY

Nitrous oxide is a permanent constituent of the atmosphere with a concentration between 0.1 and 0.3 parts per million in the troposphere. Several infrared absorption bands of this gas have been observed in atmospheric spectra. The work reported here has been directed toward the eventual tabulation of all N_2O absorption lines sufficiently intense to provide significant absorption over a straight-line path tangent to the earth's surface and extending from above the atmosphere down to the surface and back up to the top of the atmosphere. Section 2 contains two extensive tables; one gives the intensities of the band systems and the other lists the constants required to calculate the positions of most of the lines of interest. These tables summarize the results of an experimental investigation performed recently in our laboratory as well as the results of several previous studies. The emphasis of the present investigation has been on the determination of the intensities of band systems and the relative intensities of separate bands within each system. Several bands not reported previously have been observed and their intensities have been measured.

Section 3 contains detailed results from the absorption bands between approximately 1585 and 4000 cm^{-1} , and Section 4 provides similar information on the bands between 530 and 760 cm^{-1} . The region between 760 and 1600 cm^{-1} has been covered in a previous report.¹ The results include spectral curves of transmittance and of the absorption coefficient. Individual lines within the many bands can be seen in the transmittance curves, and unusual features of the curves are discussed.

Appendix A contains abstracts and errata for all of the technical reports published previously on the present contract.

DEFINITIONS, SYMBOLS AND NOMENCLATURE

The absorber thickness, u , of a gas sample is given by

$$\begin{aligned} u(\text{molecules/cm}^2) &= 2.69 \times 10^{19} p^*(\text{atm}) L(\text{cm}) (273/\theta) \\ &= 7.34 \times 10^{21} p^* L/\theta. \end{aligned} \quad (1-1)$$

The temperature θ is in degrees Kelvin, and L is the geometrical path length through the sample. The density-equivalent-pressure p^* of the absorbing gas approaches its pressure p at low pressures. Because of the non-linear relationship between the density and the pressure of a gas, p^* may differ significantly from p at high pressures. For the pressures used in the present investigation, the following expression is sufficiently accurate: $p^* = p(1 + c p)$. The pressures are in atm and, near room temperature, $c = 0.005$ for N_2O . For the largest N_2O samples studied, p^* is only approximately 5 percent greater than p ; in many of the samples, the difference is negligible. The partial pressure of N_2O is always denoted by p , and in mixtures of N_2O plus another gas species, usually N_2 , P represents the total pressure. An equivalent pressure P_e , which is proportional to the half-widths of the absorption lines, is defined below.

The true transmittance that would be observed with infinite resolving power is given by

$$T' = \exp(-u\kappa), \quad \text{or} \quad (-1/u) \ln T' = \kappa, \quad (1-2)$$

where κ is the absorption coefficient. Because of the finite slitwidth of a spectrometer and variations in κ with wavenumber due to line structure, the observed transmittance T may differ from T' at the same wavenumber. The quantity T represents a weighted average of T' over the interval passed by the spectrometer.

The absorption coefficient due to a single collision-broadened absorption line at a point within a few cm^{-1} of the line center, ν_0 , is given by the Lorentz shape:

$$k = \frac{S_J}{\pi} \frac{\alpha}{(\nu - \nu_0)^2 + \alpha^2} \quad (1-3)$$

Most of the samples in the present study were at sufficiently high pressures that collision broadening is dominant. At pressures less than approximately 0.01 atm, the more complex Voigt profile is appropriate. It has been shown^{1,2,3} that for $|\nu - \nu_0|$ greater than a few cm^{-1} , the Lorentz equation is not correct; however, it is probably adequate for most of the samples and spectral regions reported here.

Although α is proportional to pressure, the line intensity is essentially independent of pressure for the conditions of the present study and is related to the single-line absorption coefficient by

$$S_J = \int k \, d\nu. \quad (1-4)$$

In many reports and papers, including ones published previously by us, S_J is called line strength. In order to conform with the majority of the workers in the field, we will hereafter refer to S_J as the intensity, not the strength. The term S_v refers to the intensity of a vibration-rotation band which contains many lines. The combined intensity of a system of bands is denoted by S_{sys} .

If essentially all of the absorption in a given spectral region results from a system of overlapping bands, we see from Eq. (1-2) that

$$S_{\text{sys}} = \int K \, d\nu = (-1/u) \int \ln T' \, d\nu. \quad (1-5)$$

When the lines are sufficiently broad or the spectral slitwidth of the instrument is sufficiently narrow, $\int \ln T \, d\nu \approx \int \ln T' \, d\nu$, and S_{sys} can be determined from the measured quantity $(-1/u) \int \ln T \, d\nu$.

LINE WIDTHS

Equivalent pressure P_e given by the following equation is a convenient parameter when dealing with N_2O absorption by mixtures of N_2O in N_2 or in air, which is approximately 80% N_2 :

$$P_e = Bp + p_{\text{N}_2} = (B-1)p + P, \quad (1-6)$$

where p , p_{N_2} , and P are the N_2O partial pressure, N_2 partial pressure, and total pressure, respectively. B is the ratio of the self-broadening ability to the broadening ability of N_2 . We note that P_e approximates P for dilute mixtures of N_2O in N_2 ($p \ll p_{\text{N}_2}$).

We have used a technique described previously⁴ to measure B for the $2\nu_1$ band of N_2O . As an example, a spectral curve was obtained for a sample consisting of 0.133 atm of pure N_2O with a path length of 416 cm. The path length was then adjusted to 1648 cm and 0.0336 atm of N_2O was introduced to the cell to produce the same absorber thickness as in the previous sample. The sample pressure was then increased by adding N_2 ; spectral curves were scanned with the sample at various pressures. At a total pressure of 0.157 atm the absorption was essentially the same as that produced by the 0.133 atm sample of pure N_2O . Since the absorber thickness and absorption were the same for both samples, the equivalent pressures were necessarily the same. By substituting the pressures into Eq. (1-6), we obtain a value of $B = 1.24$ for this measurement.

This experiment was repeated at several different combinations of pressures and path lengths. Longer paths and relatively high pressures provided information in the regions of minimum absorption between the lines; shorter paths and lower pressures were more useful near the line centers. The results indicated that

$$B = 1.24 \pm 0.06$$

gives the best fit of the data in the regions between the lines as well as near the line centers. Since the same value of B fits both regions, we conclude that a self-broadened N_2O line has approximately the same shape as an N_2 -broadened line over the region from its center out to approximately 20.5 cm^{-1} , the distance from a line center to the point midway between it and the adjacent line.

Approximately the same N_2 pressure was required to match the absorption by the sample over the entire region from the P23 line to the R40 line of the $2\nu_1$ band, indicating that the same value of B applies over all of this region. The region beyond these lines showed little absorption and was not investigated. For most purposes it can probably be assumed that the self-broadening coefficient is independent of rotational quantum number J and is the same for all N_2O bands. The value of B determined by the present investigation is larger⁵ than the value (1.12 ± 0.07) reported by Burch, Singleton, and Williams. The more recent value, 1.24 ± 0.06 is probably more reliable because of improved gas-handling techniques. The earlier work by BSW was on the very strong ν_1 and ν_3 bands for which small samples were required. Since the $2\nu_1$ band used in the present investigation is much weaker than the ν_1 and ν_3 bands, larger samples, which could be mixed and measured more accurately, were employed.

Toth⁶ has measured the half-widths of several of the lines of the 10^0_1 and 02^0_1 bands when the lines are self broadened as well as when they are N_2 broadened. From Toth's published values of the normalized half-widths corresponding to 1 atm pressure, we have calculated the ratio $\alpha_s^0(\text{self})/\alpha_{N_2}^0$,

which corresponds to our coefficient B defined by Eq. (1-6) above. Toth's results indicate that B varies from 1.44 at $J = 20$ to 1.20 at $J = 40$. This variation in B with J is not consistent with our results discussed in the previous paragraph. The method employed by Toth provides information about the absolute value of the line half-widths, whereas, our method does not. However, our method should provide a more accurate means of determining the ratio of the broadening abilities since it is much less subject to errors introduced by weak, overlapping lines, errors in the assumed line intensities, or misplacement of the zero-absorptance curve on the spectrum.

Until further work on N_2O line half-widths is done, we recommend that Toth's values for N_2 broadening be applied to atmospheric problems with the assumption that $\alpha_{N_2}^O$ depends on J but is the same for a given J within any branch of any band. We further recommend that Toth's values of α_N^O be used with an equivalent pressure P_e given by Eq. (1-6) with $B = 1.24$ when dealing with samples in which the N_2O partial pressure is not much less than the total pressure.

SECTION 2

BAND SYSTEMS

The three fundamental bands of N_2O , ν_1 , ν_2 , and ν_3 are at 1284.907, 588.767, and 2223.756 cm^{-1} , respectively. Note that $\nu_3 \approx 2\nu_1 \approx 4\nu_2$. The quantity N defined as $2\nu_1 + \nu_2 + 4\nu_3$, where the ν 's are the vibrational quantum numbers, is convenient in specifying energy levels and in estimating band positions. Because of the approximate relationship between ν_1 , ν_2 , and ν_3 , levels having the same N are approximately equal. The changes in the quantum numbers ν_1 , ν_2 , and ν_3 during the transition are denoted by $\Delta\nu_1$, $\Delta\nu_2$, and $\Delta\nu_3$, respectively. It follows that bands arising from transitions for which $\Delta N = 2\Delta\nu_1 + \Delta\nu_2 + 4\Delta\nu_3$ is constant all occur near each other.

Each band system contains a main band and associated difference bands that arise from transitions from excited energy levels with the same changes in the vibrational quantum numbers as the main band. For example, the 00^01 band is the main one in a system that also contains the difference bands $01^11 \leftarrow 01^10$, $02^01 \leftarrow 02^00$, $02^21 \leftarrow 02^20$, $10^01 \leftarrow 10^00$, and many others from higher excited energy levels. The relative intensities of the difference bands decrease with increasing height of the lower energy level because of the decrease in its population. Corresponding bands of the rare isotopic molecules are also a part of the system.

Measuring the parameters of each individual absorption line is not possible. Many of the lines overlap each other and are too close to be resolved by spectrometers. The line parameters are being determined by a combination of experiment and theory. The intensity of a band system is determined experimentally from spectral curves of $(-1/u) \ln T$ similar to those shown in Sections 3 and 4. In many cases, the vibration-rotation interaction does not influence the line intensities significantly

and the intensity of an individual line can be calculated accurately by simple theoretical expressions from the intensity of the entire vibration-rotation band to which it belongs. The relative intensities of the lines within a band have been tabulated by Young⁷ for several types of bands for which there are negligible interactions that influence the relative intensities.

The relative intensities of the bands within several of the band systems can be estimated on the basis of the degeneracy and the relative populations of the lower energy levels involved in the transition. Thus, within one of these band systems, the intensities of the individual lines can be calculated from the experimentally determined intensity of the band system. However, the relative intensities of many of the bands can not be predicted by the simple theory because of interactions that modify the relative intensities. A considerable portion of the present study has been devoted to investigations of the relative intensities of the main bands and their associated difference bands. These investigations are continuing, and the results will be reported in the future.

Table 2-1 summarizes all of the band systems to be included in the line parameter tabulation as well as several other weaker band systems observed or looked for during the investigation. Each band system is identified by the main band in the system. The center position and the upper and lower energy levels correspond to the main band. The changes in each of the quantum numbers v_1 , v_2 , and v_3 are constant within a system, but the change in ℓ may be either 0 or ± 1 . Three forbidden bands (02^2_0 , 12^2_0 , and 06^2_0) for which $\Delta \ell = 2$ are also included; of these only the 02^2_0 band and the R27 and P29 lines of the 06^2_0 band is sufficiently intense for the line parameter tabulation. The intensities of these 06^2_0 lines are enhanced due to Fermi interaction and are discussed later.

The isotopes are indicated in the final column by 456, 546, 448, and 447 for the $^{14}\text{N}^{15}\text{N}^{16}\text{O}$, $^{15}\text{N}^{14}\text{N}^{16}\text{O}$, $^{14}\text{N}^{14}\text{N}^{18}\text{O}$, and $^{14}\text{N}^{14}\text{N}^{17}\text{O}$ molecules, respectively. Levels listed without reference to a particular isotope correspond to the most abundant isotopic molecule $^{14}\text{N}^{14}\text{N}^{16}\text{O}$.

To illustrate the notation, the line parameters in the following bands are to be included for the system containing the $01^1_0-00^0_0$ band: $01^1_0-00^0_0$, $02^0_0-01^1_0$, $02^2_0-01^1_0$, $03^1_0-02^0_0$, $03^1_0-02^2_0$, $03^3_0-02^2_0$, and the Q-branch only of $11^1_0-10^0_0$ band for the 446 isotope. Also included are the $01^1_0-00^0_0$ bands for the 456, 546, and 448 isotopes and the Q-branch only of this band for the 447 isotope. All of the lines of bands in this system that arise from energy levels higher than those listed are too weak to include in the line parameter listing. The present investigation has included measurements over the spectral region from approximately 530 cm^{-1} to above 8000 cm^{-1} ; no bands with intensity greater than $0.2 \times 10^{-20}\text{ molecules}^{-1}\text{cm}^2\text{cm}^{-1}$ other than those listed in Table 2-1 occur in this spectral region at room temperature or below.

TABLE 2-1
SUMMARY OF BAND SYSTEMS

Center of main band (cm ⁻¹)	Vibrational quantum Nos. upper lower changes level level v ₁ , v ₂ , ℓ, v ₃			Intensity of band system (multiply by 10 ⁻²⁰ molecules ⁻¹ cm ² cm ⁻¹)	Lower level of bands in parameter table and miscellaneous remarks
<u>ΔN = 1</u>					
588.767	01 ¹ 0	00 ⁰ 0	0, 1, <u>+</u> 1, 0	117.9 ± 9 122±16(8W), 147(TWW), 131(Ha), 77.5(EC), 75.2(WK), 153(G), 135(YP)	00 ⁰ 0, 01 ¹ 0, 02 ⁰ 0, 02 ² 0, 10 ⁰ 0(Q only). <u>456</u> , <u>546</u> , <u>448</u> , 00 ⁰ 0. <u>447</u> , 00 ⁰ 0(Q only).
696.140	10 ⁰ 0	01 ¹ 0	1, -1, -1, 0	0.354 ± 0.02	01 ¹ 0.
<u>ΔN = 2</u>					
938.849	00 ⁰ 1	10 ⁰ 0	-1, 0, 0, 1	0.254±0.010	10 ⁰ 0.
1037.66	04 ⁰ 0	10 ⁰ 0	-1, <u>+</u> , 0, 0	< 0.01	None.
1055.622	00 ⁰ 1	02 ⁰ 0	0, -2, 0, 1	0.054±0.004	None.
1168.134	02 ⁰ 0	00 ⁰ 0	0, 2, 0, 0	38.5±1.5, 40.5(GW), 31(EC), 44.1±4.1(8W)	00 ⁰ 0, 01 ¹ 0, 02 ⁰ 0, 02 ² 0.
1177.750	02 ² 0	00 ⁰ 0	0, 2, 2, 0		00 ⁰ 0
1284.907	10 ⁰ 0	00 ⁰ 0	1, 0, 0, 0	996±40, 975(GW), 1410(TWW), 910(EC), 980(Ha), 809(WK)	00 ⁰ 0, 01 ¹ 0, 02 ⁰ 0, 02 ² 0, 10 ⁰ 0, 03 ¹ 0, 03 ³ 0, 11 ¹ 0. <u>456</u> , <u>546</u> , <u>448</u> , 00 ⁰ 0, 01 ¹ 0. <u>447</u> , 00 ⁰ 0. Not all bands were observed because of overlapping.
<u>ΔN = 3</u>					
1634.989	00 ⁰ 1	01 ¹ 0	0, -1, -1, 1	0.278±0.02	00 ⁰ 0.
1749.058	03 ¹ 0	00 ⁰ 0	0, 3, +1, 0	0.241±0.02	00 ⁰ 0.
1880.268	11 ¹ 0	00 ⁰ 0	1, 1, <u>+</u> 1, 0	1.66±0.08, 1.51(EC)	00 ⁰ 0, 01 ¹ 0(Q only).
1974.571	20 ⁰ 0	01 ¹ 0	2, -1, <u>+</u> 1, 0	S _Q =0.024±0.002	01 ¹ 0(Q only).
<u>ΔN = 4</u>					
2079.067	02 ⁰ 1	10 ⁰ 0	-1, 2, 0, 1	< 0.002	None. May be in structure obs. near 2060 cm ⁻¹ .
2181.66	06 ⁰ 0	10 ⁰ 0	-1, 6, 0, 0	< 0.2	None. Not obs. Overlaps 00 ⁰ 1 system.
2223.756	00 ⁰ 1	00 ⁰ 0	0, 0, 0, 1	5710±250, 6870±700(8W), 5620(Ha), 6940(TWW), 6130(EC), 6010(CMT) 6500(Hu), 3700(WK), 7130(YFS), 6310(GO)	00 ⁰ 0, 01 ¹ 0, 02 ⁰ 0, 02 ² 0, 10 ⁰ 0, 03 ¹ 0, 03 ³ 0, 11 ¹ 0. <u>456</u> , <u>546</u> , <u>448</u> , <u>447</u> , 00 ⁰ 0, 01 ¹ 0.
2312.687	10 ⁰ 1	02 ⁰ 0	1, -2, 0, 1	< 0.05	None. Not obs. Overlaps 04 ⁰ 0 system.
2322.624	04 ⁰ 0	00 ⁰ 0	0, 4, 0, 0	2.7±0.3	00 ⁰ 0, 01 ¹ 0.
2461.998	12 ⁰ 0	00 ⁰ 0	1, 2, 0, 0	33.4±1.5, 37.1(V), 42.5±5.7(8W)	00 ⁰ 0, 01 ¹ 0, 02 ⁰ 0, 02 ² 0.
2474.785	12 ² 0	00 ⁰ 0	1, 2, 2, 0		none
2563.341	20 ⁰ 0	00 ⁰ 0	1, 0, 0, 0	135±7, 132(V), 173(O), 163±18(8W)	00 ⁰ 0, 01 ¹ 0, 02 ⁰ 0, 02 ² 0, 10 ⁰ 0. <u>456</u> , <u>546</u> , <u>448</u> , 00 ⁰ 0.
2668.239	30 ⁰ 0	02 ⁰ 0	3, -2, 0, 0	< 0.005	None. Obs.

TABLE 2-1 (Cont.)
SUMMARY OF BAND SYSTEMS

Center of main band (cm ⁻¹)	Vibrational quantum Nos. upper lower level level changes v ₁ , v ₂ , ℓ, v ₃			Intensity of band system (multiply by 10 ⁻²⁰ molecules ⁻¹ cm ² cm ⁻¹).	Lower level of bands in parameter table and miscellaneous remarks
<u>ΔN = 5</u>					
2798.290	01 ¹ 1	00 ⁰ 0	0, 1, +1, 1	9.62±0.96, 9.00(EC)	00 ⁰ 0, 01 ¹ 0, 02 ⁰ 0(Q only), 02 ² 0(Q only).
2892.054	10 ⁰ 1	01 ¹ 0	1, -1, -1, 1	S _P =0.009, S _R =0.007, S _Q =0.015	None. Intensities of branches, ± 10%.
2897.78	05 ¹ 0	00 ⁰ 0	0, 5, 1, 0	S _Q < 0.0013	None. Q-obs. Overlaps 10 ⁰ 1-01 ¹ 0.
3046.213	13 ¹ 0	00 ⁰ 0	1, 3, 1, 0	< 0.025	None. Obs.
3165.857	21 ¹ 0	00 ⁰ 0	2, 1, 1, 0	S _P =0.004±0.002, S _R =0.027±0.003, S _Q =0.012±0.001	None.
3247.606	30 ⁰ 0	01 ¹ 0	3, -1, -1, 0	< 0.003.	None. Obs.
<u>ΔN = 6</u>					
3363.974	02 ⁰ 1	00 ⁰ 0	0, 2, 0, 1	10.6±0.5, 6.86(V), 8.15(T)	00 ⁰ 0, 01 ¹ 0. Value by (T) determined from S _V (02 ⁰ 1) = 7.23
(T)3465.95	06 ⁰ 0	00 ⁰ 0	0, 6, 0, 0	0.0375(T)	Not Obs. Overlaps 10 ⁰ 1 band. Only lines R45 and p47 are important.
(T)3474.65	06 ² 0	00 ⁰ 0	0, 6, 0, 2		Not obs. Only lines R27 and P29 are important
3480.821	10 ⁰ 1	00 ⁰ 0	1, 0, 0, 1	197±10, 170(V), 169(T)	00 ⁰ 0, 01 ¹ 0, 02 ⁰ 0, 02 ² 0, 10 ⁰ 0. 456, 546, 448, 00 ⁰ 0. Value by (T) determined from S _V (10 ⁰ 1) = 150.
3620.941	14 ⁰ 0	00 ⁰ 0	1, 4, 0, 0	0.56 ^{+0.02} _{-0.05}	00 ⁰ 0.
3748.252	22 ⁰ 0	00 ⁰ 0	2, 2, 0, 0	4.12±0.2	00 ⁰ 0, 01 ¹ 0.
3836.373	30 ⁰ 0	00 ⁰ 0	3, 0, 0, 0	8.15±0.4	00 ⁰ 0, 01 ¹ 0.
<u>ΔN = 7</u>					
3931.258	03 ¹ 1	00 ⁰ 0	0, 3, 1, 1	0.01 ± ^{0.02} _{0.007}	None.
(4037.13)	07 ¹ 0	00 ⁰ 0	0, 7, 1, 0	< 0.005	None. Not apparent. Overlaps 11 ¹ 1 band.
4061.979	11 ¹ 1	00 ⁰ 0	1, 1, 1, 1	0.111 ± 0.006	None.
4197.960	15 ¹ 0	00 ⁰ 0	1, 5, 1, 0	< 0.005	None. Not obs.
4335.798	23 ¹ 0	00 ⁰ 0	2, 3, 1, 0	0.1 ± ^{0.1} _{0.07}	None.
4446.379	31 ¹ 0	00 ⁰ 0	3, 1, 1, 0	< 0.01	None. Q obs.
<u>ΔN = 8</u>					
4417.379	00 ⁰ 2	00 ⁰ 0	0, 0, 0, 2	6.9 ± 0.7, 6.34(V), 5.20(M)	00 ⁰ 0, 01 ¹ 0
4491.541	04 ⁰ 1	00 ⁰ 0	0, 4, 0, 1	0.02 ± ^{0.02} _{0.01}	None.
4601.80	08 ⁰ 0	00 ⁰ 0	0, 8, 0, 0	< 0.1	None. Not obs.
4630.164	12 ⁰ 1	00 ⁰ 0	1, 2, 0, 1	0.68 ± 0.07	00 ⁰ 0.
4730.828	20 ⁰ 1	00 ⁰ 0	2, 0, 0, 1	4.4 ± 0.4, 3.63(V)	00 ⁰ 0, 01 ¹ 0.
4767.13	16 ⁰ 0	00 ⁰ 0	1, 6, 0, 0	< 0.2	None. Not obs.
4911.06	24 ⁰ 0	00 ⁰ 0	2, 4, 0, 0	0.065 ± 0.007	None.
5026.34	32 ⁰ 0	00 ⁰ 0	3, 2, 0, 0	0.29 ± 0.04	00 ⁰ 0.
5105.65	40 ⁰ 0	00 ⁰ 0	4, 0, 0, 0	0.29 ± 0.03	00 ⁰ 0.

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The final two columns also include the information about the intensities of several bands too weak to include in the listing. "None" in the last column indicates that none of the bands in a system are intense enough to be included. Upper limits on the intensities of some of these bands have been established, either by estimations based on spectral features observed, or by calculating the maximum intensity that the system could have without producing observable features in the spectral curves obtained. "Not obs." or "Obs." indicates whether or not the lines within the band were observed and identified. In some cases, the absorption features may have not been observed because they overlap other bands.

Table 2-2 contains the information available to calculate the positions of the lines of most of the bands to be included in the line parameter table. Each energy level for $\ell > 0$ is split into two components; this is indicated by the c and d in the notation. The group of lines corresponding to each of the split levels is treated as a separate sub-band, although the levels are essentially coincident for small values of the rotational quantum number J. Spaces have been left blank where the information has not yet been obtained or is not known to the authors. Unless there is a footnote indicating otherwise, these values are based on three articles by Pliva.^{8,9,10} The asterisks denote constants derived from the results of several experimental programs, including the one performed in our laboratory by Dr. William S. Benedict.¹¹ The line positions can be determined from the tabulated constants by use of the following two equations:

$$\begin{aligned} \nu_0(J'') &= \nu_c + (B' + B'')m + [(B' - B'') - (D' - D'')]m^2 - [2(D' + D'') + (H' - H'')]m^3 \\ &\quad - [(D' - D'') - 3(H' - H'')]m^4 + 3(H' + H'')m^5 + (H' - H'')m^6. \end{aligned} \quad (2-1)$$

where parameters with single primes are associated with the upper energy state of the transition and parameters with double primes with the lower energy state, and $m = -J''$ for P branch ($\Delta J = 1$), $m = J'' + 1$ for R branch ($\Delta J = +1$), ν_c = band center in cm^{-1} .

For the Q Branch ($\Delta J = 0$, $m = J''$)

$$\begin{aligned} \nu_0(J'') &= \nu_c + (B' - B'')m + [(B' - B'' - (D' - D''))m^2 - [2(D' - D'') - (H' - H'')]m^3 \\ &\quad - [(D' - D'') - 3(H' - H'')]m^4 + 3(H' - H'')m^5 + (H' - H'')m^6. \end{aligned} \quad (2-2)$$

The first line to appear in each branch is indicated. If an entire branch is missing for a particular sub-band, it is indicated by "none." As an example, the P-branch of the $01^1\text{C}_0-00^0\text{O}$ sub-band starts with $J'' = 2$ (P2), there is no Q-branch, and the R-branch starts with $J'' = 0$ (R0); whereas, the $01^1\text{d}_0-00^0\text{O}$ sub-band has only the Q-branch starting with $J'' = 1$ (Q1).

TABLE 2-2
N₂O BAND PARAMETERS

Band No.	Band Center ν_c (cm ⁻¹)	Vibrational Levels			Iso- tope	Minimum J'' value in each branch			B' (cm ⁻¹)	B'-B'' Multiply by E-3 (cm ⁻¹)	D'' Multiply by E-7 (cm ⁻¹)	D'-D'' Multiply by E-7 (cm ⁻¹)	H'' Multiply by E-12 (cm ⁻¹)	H'-H'' Multiply by E-12 (cm ⁻¹)
		Notation		Energy Lower (cm ⁻¹)		P	Q	R						
		Upper	Lower											
588.767		01 ^{1c} ₀	00 ⁰ ₀	0	446	2	None	0	0.4190113	0.1664	1.795	-0.01	1.17	0
"		01 ^{1d} ₀	00 ⁰ ₀	0	"	None	1	None	0.4190113	0.9582	1.795	-0.01	"	0
579.367		02 ⁰ ₀	01 ^{1c} ₀	588.767	"	1	None	1	0.4191777	0.7416	1.785	0.660	"	0
"		02 ⁰ ₀	01 ^{1d} ₀	"	"	None	1	None	0.4199695	-0.0502	1.785	0.660	"	0
588.983		02 ^{2c} ₀	01 ^{1c} ₀	"	"	3	None	1	0.4191777	0.9476	1.785	-0.620	"	0
"		02 ^{2d} ₀	01 ^{1c} ₀	"	"	None	2	None	0.4191777	0.9476	1.785	0.010	"	0
"		02 ^{2c} ₀	01 ^{1d} ₀	"	"	None	2	None	0.4199695	0.1558	1.785	-0.620	"	0
"		02 ^{2d} ₀	01 ^{1d} ₀	"	"	3	None	1	0.4199695	0.1558	1.785	0.010	"	0
580.924		03 ^{1c} ₀	02 ⁰ ₀	1168.134	"	2	None	0	0.4199193	-0.3130	2.445	-0.250	"	0
"		03 ^{1d} ₀	02 ⁰ ₀	"	"	None	1	None	0.4199193	1.1690	2.445	-0.250	"	0
571.308*		03 ^{1c} ₀	02 ^{2c} ₀	1177.750	"	2	None	2	0.4201253	-0.5190	1.165	1.030	"	0
"		03 ^{1d} ₀	02 ^{2c} ₀	"	"	None	2	None	0.4201253	0.9630	1.165	1.030	"	0
"		03 ^{1c} ₀	02 ^{2d} ₀	"	"	None	2	None	0.4201253	-0.5190	1.795	0.400	"	0
"		03 ^{1d} ₀	02 ^{2d} ₀	"	"	2	None	2	0.4201253	0.9630	1.795	0.400	"	0
589.208		03 ^{3c} ₀	02 ^{2c} ₀	"	"	4	None	2	0.4201253	0.549*	1.165	0.64*	"	-1.03*
"		03 ^{3d} ₀	02 ^{2c} ₀	"	"	None	3	None	0.4201253	0.549*	1.165	0.64*	"	1.03*
"		03 ^{3c} ₀	02 ^{2d} ₀	"	"	None	3	None	0.4201253	0.549*	1.795	0.01*	"	-1.03*
"		03 ^{3d} ₀	02 ^{2d} ₀	"	"	4	None	2	0.4201253	0.549*	1.795	0.01*	"	1.03*
595.361		11 ^{1c} ₀	10 ⁰ ₀	1284.907	"	2	None	0	0.4172563	0.2110	1.775	-0.010	"	0
"		11 ^{1d} ₀	10 ⁰ ₀	"	"	None	1	None	0.4172563	1.1240	1.775	0	"	0
585.320		01 ^{1c} ₀	00 ⁰ ₀	0	546	2	None	0	0.404856	0.174	1.65	0	"	0
"		01 ^{1d} ₀	00 ⁰ ₀	"	546	None	1	None	0.404856	0.916	1.65	0	"	0
575.5*		01 ^{1c} ₀	00 ⁰ ₀	"	456	2	None	0	0.4189821*	0.113*	1.75*	0*	"	0
"		01 ^{1d} ₀	00 ⁰ ₀	"	456	None	1	None	0.4189821*	0.909*	1.75*	0*	"	0
586.3*		01 ^{1c} ₀	00 ⁰ ₀	"	447	2	None	0	0.406691*	0.1694*	1.72*	0*	"	0
"		01 ^{1d} ₀	00 ⁰ ₀	"	447	None	1	None	0.406691*	0.919*	1.72*	0*	"	0
584.1*		01 ^{1c} ₀	00 ⁰ ₀	"	448	2	None	0	0.395577*	0.172*	1.65*	0*	0*	0*
"		01 ^{1d} ₀	00 ⁰ ₀	"	448	None	1	None	0.395577*	0.884*	1.65*	0*	0*	0*
696.140		10 ⁰ ₀	01 ^{1c} ₀	588.767	446	1	None	1	0.4191777	-1.9214	1.785	-0.010	1.17	0
"		10 ⁰ ₀	01 ^{1d} ₀	"	"	None	1	None	0.4199695	-2.7132	1.785	-0.010	"	0
938.849		00 ⁰ ₁	10 ⁰ ₀	1284.907	"	1	None	0	0.4173163	-1.695	1.775	0.02	"	0
1168.134		02 ⁰ ₀	00 ⁰ ₀	0	"	1	None	0	0.4190113	0.9080	1.795	0.650	"	0
1160.291		03 ^{1c} ₀	01 ^{1c} ₀	588.767	"	2	None	1	0.4191777	0.4286	1.785	0.410	"	0
"		03 ^{1d} ₀	01 ^{1c} ₀	"	"	None	1	None	0.4191777	1.9106	1.785	0.410	"	0
"		03 ^{1c} ₀	01 ^{1d} ₀	"	"	None	1	None	0.4199695	-0.3632	1.785	0.410	"	0
"		03 ^{1d} ₀	01 ^{1d} ₀	"	"	2	None	1	0.4199695	1.1188	1.785	0.410	"	0
1154.436		04 ⁰ ₀	02 ⁰ ₀	1168.134	"	1	None	0	0.4199193	0.6920	2.445	1.650	"	0
1153.40		04 ^{2c} ₀	02 ^{2c} ₀	1177.750	"	3	None	2	0.4201253	0.886*	1.165	0.185*	"	0*
"		04 ^{2d} ₀	02 ^{2c} ₀	"	"	None	2	None	0.4201253	0.886*	1.165	1.085*	"	0*
"		04 ^{2c} ₀	02 ^{2d} ₀	"	"	None	2	None	0.4201253	0.886*	1.795	-0.445*	"	0*
"		04 ^{2d} ₀	02 ^{2d} ₀	"	"	3	None	2	0.4201253	0.886*	1.795	0.705*	"	0*
1177.750		02 ^{2c} ₀	00 ⁰ ₀	0	"	3	None	1	0.4190113	1.114	1.795	-0.765*	"	0
1284.907		10 ⁰ ₀	00 ⁰ ₀	0	"	1	None	0	0.4190113	-1.7550	1.795	-0.020	"	0
1291.501		11 ^{1c} ₀	01 ^{1c} ₀	588.767	"	2	None	1	0.4191777	-1.7104	1.785	-0.020	"	0
"		11 ^{1d} ₀	01 ^{1c} ₀	"	"	None	1	None	0.4191777	-0.7974	1.785	-0.010	"	0
"		11 ^{1c} ₀	01 ^{1d} ₀	"	"	None	1	None	0.4199695	-2.5022	1.785	-0.020	"	0
"		11 ^{1d} ₀	01 ^{1d} ₀	"	"	2	None	1	0.4199695	-1.5892	1.785	-0.010	"	0
1293.864		12 ⁰ ₀	02 ⁰ ₀	1168.134	"	1	None	0	0.4199193	-1.7710	2.445	0.020	"	2.60
1297.035		12 ^{2c} ₀	02 ^{2c} ₀	1177.750	"	3	None	2	0.4201253	-1.411	1.165	0.045*	"	0
"		12 ^{2d} ₀	02 ^{2c} ₀	"	"	None	2	None	0.4201253	-1.411	1.165	0.535*	"	0
"		12 ^{2c} ₀	02 ^{2d} ₀	"	"	None	2	None	0.4201253	-1.411	1.795	-0.585	"	0
"		12 ^{2d} ₀	02 ^{2d} ₀	"	"	3	None	2	0.4201253	-1.411	1.795	-0.095	"	0

TABLE 2-2 (Cont.)
N₂O BAND PARAMETERS

Band Center ν_c (cm ⁻¹)	Vibrational Levels			Iso- tope	Minimum J'' value in each branch			B'' (cm ⁻¹)	B'-B'' Multiply by E-3 (cm ⁻¹)	D'' Multiply by E-7 (cm ⁻¹)	O'-D'' Multiply by E-7 (cm ⁻¹)	H'' Multiply by E-12 (cm ⁻¹)	H'-H'' Multiply by E-12 (cm ⁻¹)
	Notation		Energy Lower (cm ⁻¹)		P	Q	R						
	Upper	Lower											
1278.434	20 ⁰ 0	10 ⁰ 0	1284.907	446	1	None	0	0.4172563	-1.6530	1.775	-0.130	1.17	0
1297.155	13 ^{1c} 0	03 ^{1c} 0	1749.058	"	2	None	1	0.4196063	-1.8430	2.195	-0.050	"	0
"	13 ^{1d} 0	03 ^{1c} 0	"	"	None	1	None	0.4196063	-0.2280	2.195	-0.030	"	0
"	13 ^{1c} 0	03 ^{1d} 0	"	"	None	1	None	0.4210883	-3.3250	2.195	-0.050	"	0
"	13 ^{1d} 0	03 ^{1d} 0	"	"	2	None	1	0.4210883	-1.7100	2.195	-0.030	"	0
1300.791*	13 ^{3c} 0	03 ^{3c} 0	1766.958*	"	4	None	3	0.42674*	-1.565*	1.805*	0*	0.14*	0.33*
"	13 ^{3d} 0	03 ^{3c} 0	"	"	None	3	None	0.42674*	-1.565*	1.805*	0*	0.14*	1.73*
"	13 ^{3c} 0	03 ^{3d} 0	"	"	None	3	None	0.42674*	-1.565*	1.805*	0*	2.20*	-1.73*
"	13 ^{3d} 0	03 ^{3d} 0	"	"	4	None	3	0.42674*	-1.565*	1.805*	0*	2.20*	-0.33*
1285.589	21 ^{1c} 0	11 ^{1c} 0	1880.268	"	2	None	1	0.4174673	-1.6340	1.765	-0.170	1.17	0
"	21 ^{1d} 0	11 ^{1c} 0	"	"	None	1	None	0.4174673	-0.5510	1.765	-0.170	"	0
"	21 ^{1c} 0	11 ^{1d} 0	"	"	None	1	None	0.4183803	-2.5470	1.775	-0.180	"	0
"	21 ^{1d} 0	11 ^{1d} 0	"	"	2	None	1	0.4183803	-1.4640	1.775	-0.180	"	0
1280.5*	10 ⁰ 0	00 ⁰ 0	0	456	1	None	0	0.4189821*	-1.79*	1.75*	-0.03*		
1286.4*	11 ^{1c} 0	01 ^{1c} 0	575.5*	456	2	None	1	0.419095*	-1.75*	1.75*	-0.04*		
"	11 ^{1d} 0	01 ^{1c} 0	"	456	None	1	None	0.419095*	-0.89*	1.75*	-0.05*		
"	11 ^{1c} 0	01 ^{1d} 0	"	456	None	1	None	0.419891*	-2.55*	1.75*	-0.04*		
"	11 ^{1d} 0	01 ^{1d} 0	"	456	2	None	1	0.419891*	-1.69*	1.75*	-0.05*		
1269.894*	10 ⁰ 0	00 ⁰ 0	0	546	1	None	0	0.4048564*	-1.587*	1.65*	-0.05*		
1277.760*	11 ^{1c} 0	01 ^{1c} 0	585.320*	546	2	None	1	0.4050304*	-1.569*	1.65*	-0.06*		
"	11 ^{1d} 0	01 ^{1c} 0	"	546	None	1	None	0.4050304*	-0.649*	1.65*	-0.08*		
"	11 ^{1c} 0	01 ^{1d} 0	"	546	None	1	None	0.4057724*	-2.311*	1.65*	-0.06*		
"	11 ^{1d} 0	01 ^{1d} 0	"	546	2	None	1	0.4057724*	-1.391*	1.65*	-0.08*		
1247.9*	10 ⁰ 0	00 ⁰ 0	0	448	1	None	0	0.395577*	-1.52*	1.65*	-0.10*		
1255.7*	11 ^{1c} 0	01 ^{1c} 0	584.1*	448	2	None	1	0.395749*	-1.45*	1.65*	-0.09*		
"	11 ^{1d} 0	01 ^{1c} 0	"	448	None	1	None	0.395749*	-0.52*	1.65*	-0.15*		
"	11 ^{1c} 0	01 ^{1d} 0	"	448	None	1	None	0.396461*	-2.16*	1.65*	-0.09*		
"	11 ^{1d} 0	01 ^{1d} 0	"	448	2	None	1	0.396461*	-1.33*	1.65*	-0.15*		
1265.5*	10 ⁰ 0	00 ⁰ 0	0	447	1	None	0	0.406691*	-0.73*	1.72*	-0.05*		
1634.989	00 ⁰ 1	01 ^{1c} 0	588.767	446	1	None	1	0.4191777	-3.6164	1.785	0.01	1.17	0
"	00 ⁰ 1	01 ^{1d} 0	"	"	None	1	None	0.4199695	-4.4002	1.785	0.01	"	0
1749.058	03 ^{1c} 0	00 ⁰ 0	0	"	2	None	0	0.4190113	0.5950	1.795	0.400	"	0
"	03 ^{1d} 0	00 ⁰ 0	"	"	None	1	None	0.4190113	2.0770	1.795	0.400	"	0
1880.268	11 ^{1c} 0	00 ⁰ 0	0	"	2	None	0	0.4190113	-1.5440	1.795	-0.030	"	0
"	11 ^{1d} 0	00 ⁰ 0	"	"	None	1	None	0.4190113	-0.6310	1.795	-0.020	"	0
1886.018	12 ^{2c} 0	01 ^{1c} 0	588.767	"	3	None	1	0.4191777	-0.4634	1.785	-0.575*	"	0
"	12 ^{2d} 0	01 ^{1c} 0	"	"	None	2	None	0.4191777	-0.4634	1.785	-0.085*	"	0
"	12 ^{2c} 0	01 ^{1d} 0	"	"	None	2	None	0.4199695	-1.2552	1.785	-0.575*	"	0
"	12 ^{2d} 0	01 ^{1d} 0	"	"	3	None	1	0.4199695	-1.2552	1.785	-0.085*	"	0
1873.231	12 ⁰ 0	01 ^{1c} 0	"	"	1	None	1	0.4191777	-1.0294	1.785	0.68	"	2.6
"	12 ⁰ 0	01 ^{1d} 0	"	"	None	1	None	0.4199695	-1.8212	1.785	0.68	"	2.6
1974.574	20 ⁰ 0	01 ^{1c} 0	"	"	1	None	1	0.4191777	-3.5744	1.785	-0.14	"	0
"	20 ⁰ 0	01 ^{1d} 0	"	"	None	1	None	0.4199695	-4.3662	1.785	-0.14	"	0
2223.756	00 ⁰ 1	00 ⁰ 0	0	"	1	None	0	0.4190113	-3.4500	1.795	0	"	0
2209.523	01 ^{1c} 1	01 ^{1c} 0	588.767	"	2	None	1	0.4191777	-3.4054	1.785	0.010	"	0
"	01 ^{1d} 1	01 ^{1c} 0	"	"	None	1	None	0.4191777	-2.6304	1.785	0.010	"	0
"	01 ^{1c} 1	01 ^{1d} 0	"	"	None	1	None	0.4199695	-4.1972	1.785	0.010	"	0
"	01 ^{1d} 1	01 ^{1d} 0	"	"	2	None	1	0.4199695	-3.4222	1.785	0.010	"	0
2195.840	02 ⁰ 1	02 ⁰ 0	1168.134	"	1	None	0	0.4199193	-3.3750	2.445	0	"	0

TABLE 2-2 (Cont.)
N₂O BAND PARAMETERS

Band Center ν_c (cm ⁻¹)	Vibrational Levels			Iso- tope	Minimum J" value in each branch			8" (cm ⁻¹)	B'-8" Multiply by E-3 (cm ⁻¹)	D" Multiply by E-7 (cm ⁻¹)	D'-D" Multiply by E-7 (cm ⁻¹)	H" Multiply by E-12 (cm ⁻¹)	H'-H" Multiply by E-12 (cm ⁻¹)
	Notation		Energy Lower (cm ⁻¹)		P	Q	R						
	Upper	Lower											
2195.387	02 ² c ₁	02 ² c ₀	1177.750	446	3	None	2	0.4201253	-3.3730	1.165	0.030	1.17	0
"	02 ² d ₁	02 ² c ₀	"	"	None	2	None	0.4201253	-3.3730	1.165	0.630	"	0
"	02 ² c ₁	02 ² d ₀	"	"	None	2	None	0.4201253	-3.3730	1.795	-0.600	"	0
"	02 ² d ₁	02 ² d ₀	"	"	3	None	2	0.4201253	-3.3730	1.795	0	"	0
2195.914	10 ⁰ 1	10 ⁰ 0	1284.907	"	1	None	0	0.4172563	-3.4720	1.775	-0.030	"	0
2182.200	03 ¹ c ₁	03 ¹ c ₀	1749.058	"	2	None	1	0.4196063	-3.3810	2.195	-0.280	"	0
"	03 ¹ d ₁	03 ¹ c ₀	"	"	None	1	None	0.4196063	-1.9220	2.195	-0.270	"	0
"	03 ¹ c ₁	03 ¹ d ₀	"	"	None	1	None	0.4210883	-4.8630	2.195	-0.280	"	0
"	03 ¹ d ₁	03 ¹ d ₀	"	"	2	None	1	0.4210883	-3.4040	2.195	-0.270	"	0
2181.386*	03 ³ c ₁	03 ³ c ₀	1766.958*	"	4	None	3	0.42674*	-3.347*	1.805*	0.01*	0.14*	0
"	03 ³ d ₁	03 ³ c ₀	"	"	None	3	None	0.42674*	-3.347*	1.805*	0.01*	0.14*	2.06*
"	03 ³ c ₁	03 ³ d ₀	"	"	None	3	None	0.42674*	-3.347*	1.805*	0.01*	2.20*	-2.06*
"	03 ³ d ₁	03 ³ d ₀	"	"	4	None	3	0.42674*	-3.347*	1.805*	0.01*	2.20*	0
2181.711	11 ¹ c ₀	11 ¹ c ₀	1880.268	"	2	None	1	0.4174673	-3.4160	1.765	0.010	1.17	0
"	11 ¹ d ₁	11 ¹ c ₀	"	"	None	1	None	0.4174673	-2.5330	1.765	-0.030	"	0
"	11 ¹ c ₁	11 ¹ d ₀	"	"	None	1	None	0.4183803	-4.3290	1.775	0	"	0
"	11 ¹ d ₁	11 ¹ d ₀	"	"	2	None	1	0.4183803	-3.4460	1.775	-0.040	"	0
2193.623	00 ⁰ 2	00 ⁰ 1	2223.756	"	1	None	0	0.4155613	-3.465	1.795	-0.030	"	0
(P) 2177.659	00 ⁰ 1	00 ⁰ 0	0	456	1	None	0	0.4189821	-3.30	1.75	0	"	0
(P) 2164.13	01 ¹ c ₁	01 ¹ c ₀	575.50*	456	2	None	1	0.419095*	-3.24*	1.75	0*	"	0
"	01 ¹ d ₁	01 ¹ c ₀	"	456	None	1	None	0.419095*	-2.59*	1.75	0*	"	0
"	01 ¹ c ₁	01 ¹ d ₀	"	456	None	1	None	0.419891*	-4.04*	1.75	0*	"	0
"	01 ¹ d ₁	01 ¹ d ₀	"	456	2	None	1	0.419891*	-3.29*	1.75	0*	"	0
(P) 2201.604	00 ⁰ 1	00 ⁰ 0	0	546	1	None	0	0.4048564	-3.37	1.65	0	"	0
2187.389	01 ¹ c ₁	01 ¹ c ₀	585.320	546	2	None	1	0.4050304	-3.325	1.65	0	"	0
"	01 ¹ d ₁	01 ¹ c ₀	"	546	None	1	None	0.4050304	-2.62*	1.65	0	"	0
"	01 ¹ c ₁	01 ¹ d ₀	"	546	None	1	None	0.4057724	-4.07	1.65	0	"	0
"	01 ¹ d ₁	01 ¹ d ₀	"	546	2	None	1	0.4057724	-3.37*	"	"	"	0
(P) 2218.97*	00 ⁰ 1	00 ⁰ 0	0	448	1	None	0	0.395577	-3.26*	1.65	0	"	0
2204.70*	01 ¹ c ₁	01 ¹ c ₀	584.1*	448	2	None	1	0.395749*	-3.20*	1.65*	"	"	0
"	01 ¹ d ₁	01 ¹ c ₀	"	448	None	1	None	0.395749*	-2.54*	1.65*	"	"	0
"	01 ¹ c ₁	01 ¹ d ₀	"	448	None	1	None	0.396461*	-3.91*	1.65*	"	"	0
"	01 ¹ d ₁	01 ¹ d ₀	"	448	2	None	1	0.396461*	-3.25*	1.65*	"	"	0
2221.3*	00 ⁰ 1	00 ⁰ 0	0	447	1	None	0	0.406691*	-3.35*	1.72*	"	"	0
2207.25*	01 ¹ c ₁	01 ¹ c ₀	586.3*	447	2	None	1	0.406860*	-3.29*	1.72*	"	"	0
"	01 ¹ d ₁	01 ¹ c ₀	"	447	None	1	None	0.406860*	-2.54*	1.72*	"	"	0
"	01 ¹ c ₁	01 ¹ d ₀	"	447	None	1	None	0.407610*	-4.08*	1.72*	"	"	0
"	01 ¹ d ₁	01 ¹ d ₀	"	447	2	None	1	0.407610*	-3.33*	1.72*	"	"	0
2322.624*	04 ⁰ 0	00 ⁰ 0	0	446	1	None	0	0.4190113	1.659*	1.795	2.8*	1.17	27.4
2309.109*	05 ¹ c ₀	01 ¹ c ₀	588.767	"	2	None	1	0.4191777	0.554*	1.785	0.30*	"	0
"	05 ¹ d ₀	01 ¹ c ₀	"	"	None	1	None	0.4191777	2.794*	1.785	0.57*	"	0
"	05 ¹ c ₀	01 ¹ d ₀	"	"	None	1	None	0.4199695	-2.338*	1.785	0.30*	"	0
"	05 ¹ d ₀	01 ¹ d ₀	"	"	2	None	1	0.4199695	0.002*	1.785	0.57*	"	0
2461.998	12 ⁰ 0	00 ⁰ 0	0	"	1	None	0	0.4190113	-0.8630	1.795	0.670	"	2.6
2457.446	13 ¹ c ₀	01 ¹ c ₀	588.767	"	2	None	1	0.4191777	-1.4144	1.785	0.360	"	0
"	13 ¹ d ₀	01 ¹ c ₀	"	"	None	1	None	0.4191777	0.2006	1.785	0.380	"	0
"	13 ¹ c ₀	01 ¹ d ₀	"	"	None	1	None	0.4199695	-2.2062	1.785	0.360	"	0
"	13 ¹ d ₀	01 ¹ d ₀	"	"	2	None	1	0.4199695	-0.5912	1.785	0.380	"	0
2452.807	14 ⁰ 0	02 ⁰ 0	1168.134	"	1	None	0	0.4199193	-1.1320	2.445	1.440	"	13.0

TABLE 2-2 (Cont.)

N₂O BAND PARAMETERS

Band Center ν_c (cm^{-1})	Vibrational Levels		Iso- tope	Minimum J" value in each branch			B" (cm^{-1})	B'-B" Multiply by E-3 (cm^{-1})	D" Multiply by E-7 (cm^{-1})	D'-D" Multiply by E-7 (cm^{-1})	H" Multiply by E-12 (cm^{-1})	H'-H" Multiply by E-12 (cm^{-1})	
	Notation	Energy		P	Q	R							
	Upper	Lower											
2453.900	14 ² c ₀	02 ² c ₀	1177.750	446	3	None	2	0.4201253	-1.111*	1.165	-0.79*	1.17	0
"	14 ² d ₀	02 ² c ₀	"	"	None	2	None	0.4201253	-1.111*	1.165	0.88*	"	0
"	14 ² c ₀	02 ² d ₀	"	"	None	2	None	0.4201253	-1.111*	1.795	-1.42*	"	0
"	14 ² d ₀	02 ² d ₀	"	"	3	None	2	0.4201253	-1.111*	1.795	0.25*	"	0
2463.345	22 ⁰ c ₀	10 ⁰ c ₀	1284.907	"	1	None	0	0.4172563	-0.929	1.775	0.62	"	0
2563.341	20 ⁰ c ₀	00 ⁰ c ₀	0	"	1	None	0	0.4190113	-3.4080	1.795	-0.150	"	0
2577.090	21 ¹ c ₀	01 ¹ c ₀	588.767	"	2	None	1	0.4191777	-3.3444	1.785	-0.190	"	0
"	21 ¹ d ₀	01 ¹ c ₀	"	"	None	1	None	0.4191777	-2.2614	1.735	-0.190	"	0
"	21 ¹ c ₀	01 ¹ d ₀	"	"	None	1	None	0.4199695	-4.1362	1.785	-0.190	"	0
"	21 ¹ d ₀	01 ¹ d ₀	"	"	2	None	1	0.4199695	-3.0532	1.785	-0.190	"	0
2580.118	22 ⁰ c ₀	02 ⁰ c ₀	1168.134	"	1	None	0	0.4199193	-3.5920	2.445	-0.050	"	0
2588.310	22 ² c ₀	02 ² c ₀	1177.750	"	3	None	2	0.4201253	-2.924	1.165	0.035*	"	0
"	22 ² d ₀	02 ² c ₀	"	"	None	2	None	0.4201253	-2.924	1.165	0.395*	"	0
"	22 ² c ₀	02 ² d ₀	"	"	None	2	None	0.4201253	-2.924	1.795	-0.595*	"	0
"	22 ² d ₀	02 ² d ₀	"	"	3	None	2	0.4201253	-2.924	1.795	-0.235*	"	0
2551.466	30 ⁰ c ₀	10 ⁰ c ₀	1284.907	"	1	None	0	0.4172563	-3.1090	1.775	-0.390	"	0
2534.21*	20 ⁰ c ₀	00 ⁰ c ₀	0	546	1	None	0	0.4048564*	-2.986*	1.65*	-0.20*	"	0
2554.3*	20 ⁰ c ₀	00 ⁰ c ₀	"	456	1	None	0	0.4189821*	-3.53*	1.75*	-0.09*	"	0
2491.3*	20 ⁰ c ₀	00 ⁰ c ₀	"	448	1	None	0	0.395557*	-2.79*	1.65*	-0.34*	"	0
2798.290	01 ¹ c ₁	00 ⁰ c ₀	"	446	2	None	0	0.4190113	-3.2390	1.795	0	1.17	0
"	01 ¹ d ₁	00 ⁰ c ₀	"	"	None	1	None	0.4190113	-2.4640	1.795	0	"	0
2775.207	02 ⁰ c ₁	01 ¹ c ₀	588.767	"	1	None	1	0.4191777	-2.6334	1.785	0.660	"	0
"	02 ⁰ c ₁	01 ¹ d ₀	"	"	None	1	None	0.4199695	-3.4252	1.785	0.660	"	0
2784.370	02 ² c ₁	01 ¹ c ₀	"	"	3	None	1	0.4191777	-2.4254	1.785	-0.590	"	0
"	02 ² d ₁	01 ¹ c ₀	"	"	None	2	None	0.4171777	-2.4254	1.785	0.010	"	0
"	02 ² c ₁	01 ¹ d ₀	"	"	None	2	None	0.4199695	-3.2172	1.785	-0.590	"	0
"	02 ² d ₁	01 ¹ d ₀	"	"	3	None	1	0.4199695	-3.2172	1.785	0.010	"	0
2763.124	03 ¹ c ₁	02 ⁰ c ₀	1168.134	446	2	None	0	0.4199193	-3.694	2.445	-0.53	"	0
"	03 ¹ d ₁	02 ⁰ c ₀	"	"	None	1	None	0.4199193	-2.235	2.445	-0.52	"	0
2753.508	03 ¹ c ₁	02 ² c ₀	1177.750	"	2	None	2	0.4201513	-3.900	1.165	0.75	"	0
"	03 ¹ d ₁	02 ² c ₀	"	"	None	2	None	0.4201253	-2.441	1.165	0.76	"	0
"	03 ¹ c ₁	02 ² d ₀	"	"	None	2	None	0.4201253	-3.900	1.795	0.12	"	0
"	03 ¹ d ₁	02 ² d ₀	"	"	2	None	2	0.4201253	-2.441	1.795	0.13	"	0
2770.594*	03 ³ c ₁	02 ² c ₀	"	"	4	None	2	0.4201253	-2.826*	1.165	0.645*	"	-1.03*
"	03 ³ d ₁	02 ² c ₀	"	"	None	3	None	0.4201253	-2.826*	1.165	0.645*	"	1.03*
"	03 ³ c ₁	02 ² d ₀	"	"	None	3	None	0.4201253	-2.826*	1.795	0.015*	"	-1.03*
"	03 ³ d ₁	02 ² d ₀	"	"	4	None	2	0.4201253	-2.826*	1.795	0.015*	"	1.03*
3363.974	02 ⁰ c ₁	00 ⁰ c ₀	0	"	1	None	0	0.4190113	-2.467	1.795	0.650	"	0
3342.491	03 ¹ c ₁	01 ¹ c ₀	588.767	"	2	None	1	0.4191777	-2.9524	1.785	0.130	"	0
"	03 ¹ d ₁	01 ¹ c ₀	"	"	None	1	None	0.4191777	-1.4934	1.785	0.140	"	0
"	03 ¹ c ₁	01 ¹ d ₀	"	"	None	1	None	0.4199695	-3.7442	1.785	0.130	"	0
"	03 ¹ d ₁	01 ¹ d ₀	"	"	2	None	1	0.4199695	-2.2852	1.785	0.140	"	0
3480.821	10 ⁰ c ₁	00 ⁰ c ₀	0	"	1	None	0	0.4190113	-5.2270	1.795	-0.050	"	0
3473.212	11 ¹ c ₁	01 ¹ c ₀	588.767	"	2	None	1	0.4191777	-5.1264	1.785	-0.010	"	0
"	11 ¹ d ₁	01 ¹ c ₀	"	"	None	1	None	0.4191777	-4.2434	1.785	-0.050	"	0
"	11 ¹ c ₁	01 ¹ d ₀	"	"	None	1	None	0.4199695	-5.9182	1.785	-0.010	"	0
"	11 ¹ d ₁	01 ¹ d ₀	"	"	2	None	1	0.4199695	-5.0352	1.758	-0.050	"	0
3462.030	12 ⁰ c ₁	02 ⁰ c ₀	1168.134	"	1	None	0	0.4199193	-5.1560	2.445	0.030	"	0

TABLE 2-2 (Cont.)
N₂O BAND PARAMETERS

Band Center ν_c (cm ⁻¹)	Vibrational Levels		Iso- tope	Minimum J" value in each branch			8"	8'-8"	D"	D'-D"	H"	H'-H"	
	Notation	Energy											
	Upper	Lower		P	Q	R							
		(cm ⁻¹)					(cm ⁻¹)	(cm ⁻¹)	(cm ⁻¹)	(cm ⁻¹)	(cm ⁻¹)	(cm ⁻¹)	
3464.713	12 ² c ₁	02 ² c ₀	1177.750	446	3	None	2	0.4201253	-4.9670	1.165	-0.15	1.17	0
"	12 ² d ₁	02 ² c ₀	"	"	None	2	None	0.4201253	-4.9670	1.165	-0.15	"	0
"	12 ² c ₁	02 ² d ₀	"	"	None	2	None	0.4201253	-4.9670	1.795	0.48	"	0
"	12 ² d ₁	02 ² d ₀	"	"	3	None	2	0.4201253	-4.9670	1.795	0.48	"	0
3445.921	20 ⁰ 1	10 ⁰ 0	1284.907	"	1	None	0	0.4172563	-5.140	1.775	-0.150	"	0
3443.659	10 ⁰ 1	00 ⁰ 0	0	546	1	None	0	0.4048564	-4.980	1.65	-0.05	"	
3430.95*	10 ⁰ 1	00 ⁰ 0	"	456	1	None	0	0.418982*	-5.11*	1.75*	-0.03*	"	
3439.1*	10 ⁰ 1	00 ⁰ 0	"	448	1	None	0	0.395577*	-4.80*	1.65*	-0.10*	"	
3466.57	06 ⁰ 0	00 ⁰ 0	0	446	1	None	0	0.4190113		1.795		1.17	0
3748.252	22 ⁰ 0	00 ⁰ 0	0	"	1	None	0	0.4190113	-2.684	1.795	0.60	"	1.60
3747.031	23 ¹ c ₀	01 ¹ c ₀	588.767	"	2	None	1	0.4191777	-3.2584	1.785	0.26	"	0
"	23 ¹ d ₀	01 ¹ c ₀	"	"	None	1	None	0.4191777	-1.4964	1.785	0.33	"	0
"	23 ¹ c ₀	01 ¹ d ₀	"	"	None	1	None	0.4199695	-4.0502	1.785	0.26	"	0
"	23 ¹ d ₀	01 ¹ d ₀	"	"	2	None	1	0.4199695	-2.2882	1.785	0.33	"	0
3620.941	14 ⁰ 0	00 ⁰ 0	0	"	1	None	0	0.4190113	-0.2240	1.795	2.090	"	0
3836.373	30 ⁰ 0	00 ⁰ 0	0	"	1	None	0	0.4190113	-4.8640	1.795	-0.410	"	0
3857.612	31 ¹ c ₀	01 ¹ c ₀	588.767	"	2	None	1	0.4191777	-4.8074	1.785	-0.16	"	0
"	31 ¹ d ₀	01 ¹ c ₀	"	"	None	1	None	0.4191777	-3.5064	1.785	-0.42	"	0
"	31 ¹ c ₀	01 ¹ d ₀	"	"	None	1	None	0.4199695	-5.5992	1.785	-0.16	"	0
"	31 ¹ d ₀	01 ¹ d ₀	"	"	2	None	1	0.4199695	-4.2982	1.785	-0.42	"	0
4417.379	00 ⁰ 2	00 ⁰ 0	0	"	1	None	0	0.4190113	-6.9150	1.795	-0.030	"	0
4388.928	01 ¹ c ₂	01 ¹ c ₀	588.767	"	2	None	1	0.4191777	-6.8194	1.785	0	"	0
"	01 ¹ d ₂	01 ¹ c ₀	"	"	None	1	None	0.4191777	-6.0594	1.785	"	"	0
"	01 ¹ c ₂	01 ¹ d ₀	"	"	None	1	None	0.4199695	-7.6112	1.785	"	"	0
"	01 ¹ d ₂	01 ¹ d ₀	"	"	2	None	1	0.4199695	-6.8512	1.785	"	"	0
4630.164	12 ⁰ 1	00 ⁰ 0	0	"	1	None	0	0.4190113	-4.2480	1.795	0.680	"	3.0
4730.828	20 ⁰ 1	00 ⁰ 0	0	"	1	None	0	0.4190113	-6.8950	1.795	-0.170	"	
4730.408	21 ¹ c ₁	01 ¹ c ₀	588.767	446	2	None	1	0.4191777	-6.7464	1.785	-0.110	"	
"	21 ¹ d ₁	01 ¹ c ₀	"	"	None	1	None	0.4191777	-5.7074	1.785	-0.230	"	
"	21 ¹ c ₁	01 ¹ d ₀	"	"	None	1	None	0.4199695	-7.5382	1.785	-0.11	"	
"	21 ¹ d ₁	01 ¹ d ₀	"	"	2	None	1	0.4199695	-6.4992	1.785	-0.23	"	
4977.695	01 ¹ c ₂	00 ⁰ 0	0	"	2	None	0	0.4190113	-6.653	1.795	-0.01	"	
"	01 ¹ d ₂	00 ⁰ 0	"	"	None	1	None	0.4190113	-5.8930	1.795	-0.01	"	
5026.34	32 ⁰ 0	00 ⁰ 0	0	"	1	None	0	0.4190113	-4.70	1.795	0	"	
5105.65	40 ⁰ 0	00 ⁰ 0	0	"	1	None	0	0.4190113	-5.82	1.795	0	"	

Footnotes and References for Table 2-2

* Values obtained from private communication with W. S. Benedict.

(P) E. K. Plyler, E. D. Tiddwell and A. G. Makl, J. Research Nat'l Bur. Standards, **68A**, 79 (1964).

(T) R. A. Toth, J. Mol. Spec., **40**, 588 (1971).

The only lines whose intensities are strong enough to consider in the 06⁰0 and 06²0 bands are the R45 and P47 and the R27 and P29, respectively. These lines are enhanced due to Fermi interaction of the 10⁰1 vibrational level with the 06⁰0 and 06²0 levels. See text.

SECTION 3

DATA ON THE 1585-4000 cm^{-1} REGION

Data presented in this section cover all of the important N_2O bands between 1585 and 4000 cm^{-1} . The experimental apparatus and procedures have been described previously. Instrument components and gases were employed for wavenumber calibration as shown in the following table for four different sub-regions:

Sub-region (cm^{-1})	Grating lines/mm λ , blaze	Detector and liquid coolant	Calibration gas
1585-1800	150, 6 μm	Ge:Hg (He)	H_2O
1800-2200	150, 6 μm	InSb (N_2)	H_2O
2200-3250	300, 3 μm	InSb (N_2)	$\text{CO}_2, \text{N}_2\text{O}, \text{H}_2\text{O}$
3250-4000	300, 3 μm	PbS (freon 13, 191 K)	$\text{N}_2\text{O}, \text{H}_2\text{O}$

A CaF_2 foreprism eliminated overlapping orders. In many cases the N_2O line positions had been measured previously by various workers and were used for wavenumber calibration. Pliva's^{8,9,10} summary articles provide the constants required to calculate the positions of many of the lines. Well-known lines of other gases were used for calibration where the N_2O line positions could not be calculated and to check the calculated N_2O positions. A few energy levels for which Pliva's constants as listed in Table 2-2 need revision are noted.

Several of the figures presented below include high-resolution spectra from which one can identify lines of the main bands and some of the "hot" bands that arise from transitions between excited energy levels. In order

to enhance the absorption by the hot bands, we heated several of the samples to approximately 400K. Several figures represent high-pressure samples for which the lines are broadened and the line structure is smoothed so that the observed transmittance T is approximately equal to the true transmittance T' . These samples provided data on $(-1/u) \ln T$ and, in turn, the intensity, $\int (-1/u) \ln T \, dv$ of the band systems. A spectral curve of $(-1/u) \ln T$ was frequently obtained from a composite of more than one high-pressure sample. A high-pressure sample with a small absorber thickness was typically scanned in order to determine accurate values for a prominent feature such as a Q-branch, whereas another high-pressure sample with larger absorber thickness provided data in the wings of the band. In general, spectra of several high-pressure samples with different absorber thicknesses were compared to determine values of $(-1/u) \ln T$. Some of the plots of $(-1/u) \ln T$ have an expanded ordinate scale to show the wings of the band more accurately.

Absorption by H_2O contaminant created a problem in the spectral region between approximately 3300 and 3900 cm^{-1} . Some H_2O remained in the spectrometer tank although it was pumped on continuously. Its absorption could readily be seen in the background curves as well as in the high-pressure samples. Since the spectrometer tank was at a low pressure, the absorption appeared as sharp lines on a smooth curve and could be accounted for easily. H_2O was also present as a contaminant in both the N_2O and in the N_2 used as a broadening gas; the very strong H_2O lines were very evident in spectra of N_2O or N_2 at 1 atm. The H_2O absorption in high-pressure samples could be recognized, but since the lines were pressure broadened the H_2O contribution could not be accounted for accurately.

We found that much of the H_2O in the samples could be removed by the following procedure. The N_2 was cooled by passing it through a coil of copper tubing immersed in liquid N_2 . The N_2O was dried by freezing it in a lecture bottle that was placed in liquid N_2 . The frozen N_2O was then allowed to warm up and evaporate into the sample cell, leaving most of the H_2O trapped in the bottle.

The following discussion is limited to the important and unusual features of the data in the spectral region from 1585 to 4000 cm^{-1} . Any sub-region not discussed has no absorption of significance. Table 2-1 summarizes the bands in each system and their intensities. Data on the positions of band centers and the branches present in each of the sub-bands are presented in Table 2-2.

1585-1675 cm^{-1}

The main absorption band ($00^0_1 \leftarrow 01^1_0$) in this region is centered at 1634.989 cm^{-1} . Line structure in the $01^1_1 \leftarrow 02^2_0$ and $01^1_0 \leftarrow 02^0_0$ bands centered near 1620.540 and 1630.156 cm^{-1} , respectively, was also observed

in spectral curves not included in this report. The prominent features of the main band can be seen in Figs. 3-1 and 3-2. The Q-branches of the hot bands can be seen, although the one near 1630 cm^{-1} is partially hidden by the Q-branch of the main band.

$1695\text{--}1795\text{ cm}^{-1}$

The main absorption band ($03^1_0\text{--}00^0_0$) in this region is centered at 1749.058 cm^{-1} . The Q-branches of the $04^0_0\text{--}01^1_0$ and $04^0_0\text{--}01^1_0$ bands centered at 1733.80 and 1742.38 cm^{-1} , respectively, are also apparent in Figs. 3-3 and 3-4.

$1820\text{--}2100\text{ cm}^{-1}$

The strongest absorption in this region is due to the system containing the 11^1_0 band centered at 1880.268 cm^{-1} . The Q-branches of two associated difference bands, $12^0_0\text{--}01^1_0$ and $12^2_0\text{--}01^1_0$ centered at 1873.231 and 1886.018 cm^{-1} are prominent in the spectral curves of Figs. 3-5 through 3-8. Other unidentified features such as the one near 1890 cm^{-1} may be Q-branches of other difference bands or of the rarer isotopes. These band systems have been reported by Plyler, Tidwell, and Maki,¹² but the intensities have not been determined previously.

The $20^0_0\text{--}01^1_0$, $21^1_0\text{--}02^2_0$, and $21^1_0\text{--}02^0_0$ bands were identified between 1920 and 2005 cm^{-1} ; their centers are at 1974.571 , 1988.197 , and 1997.723 cm^{-1} , respectively. The main feature in this region is the Q-branch of the $20^0_0\text{--}01^1_0$ band. Note that Δv_2 is negative (-1) in this band system.

The spectral region from $2005\text{--}2100\text{ cm}^{-1}$ was examined to try to locate the $02^0_1\text{--}10^0_0$ band at 2079.067 cm^{-1} . Some weak lines observed between 2079 and 2050 cm^{-1} in a spectrum of a sample at 373K with $u = 3200 \times 10^{20}$ molecules/ cm^2 may be attributed to the P-branch of this band. The absorbance at the center of the strongest line was approximately 2 percent. From the equivalent width of the strongest lines, we determined that the intensity of the band could not be greater than 0.0002×10^{-20} molecules/ $\text{cm}^2\text{ cm}^{-1}$.

$2100\text{--}2260\text{ cm}^{-1}$

The very strong band ($00^0_1\text{--}00^0_0$) in this region is centered at 2223.756 cm^{-1} . Figures 3-9 and 3-10 show high-resolution transmittance curves for three samples at relatively low pressures so that the line structure is retained. The influence of the associated difference bands is apparent. Figure 3-11 shows transmittance curves between 2100 and 2380 cm^{-1} for a variety of high-pressure samples with the line structure smoothed. The transmittance maximum near 2322 cm^{-1} is at the center of the $04^0_0\text{--}00^0_0$ band which is discussed below. Figures 3-13 and 3-14 are plots of transmittance obtained

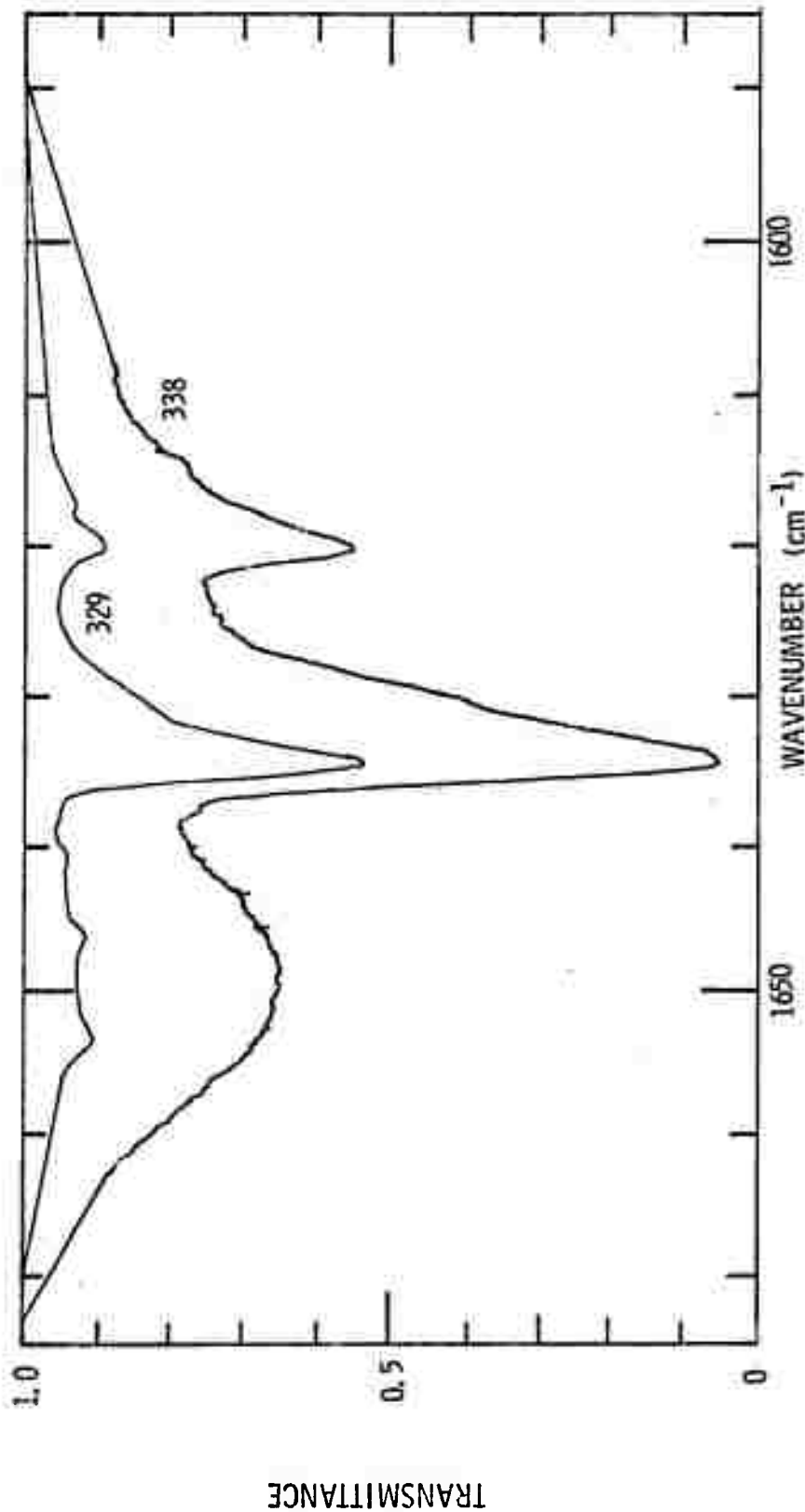


FIG. 3-1. Spectral curves of transmittance from 1585 to 1675 cm^{-1} .

Sample No.	p	P	L	u
	atm	atm	cm	molecules/ cm^2
338	1.0	8.0	416	$103.7 \text{ E } 20$
329	0.197	8.0	416	$20.4 \text{ E } 20$

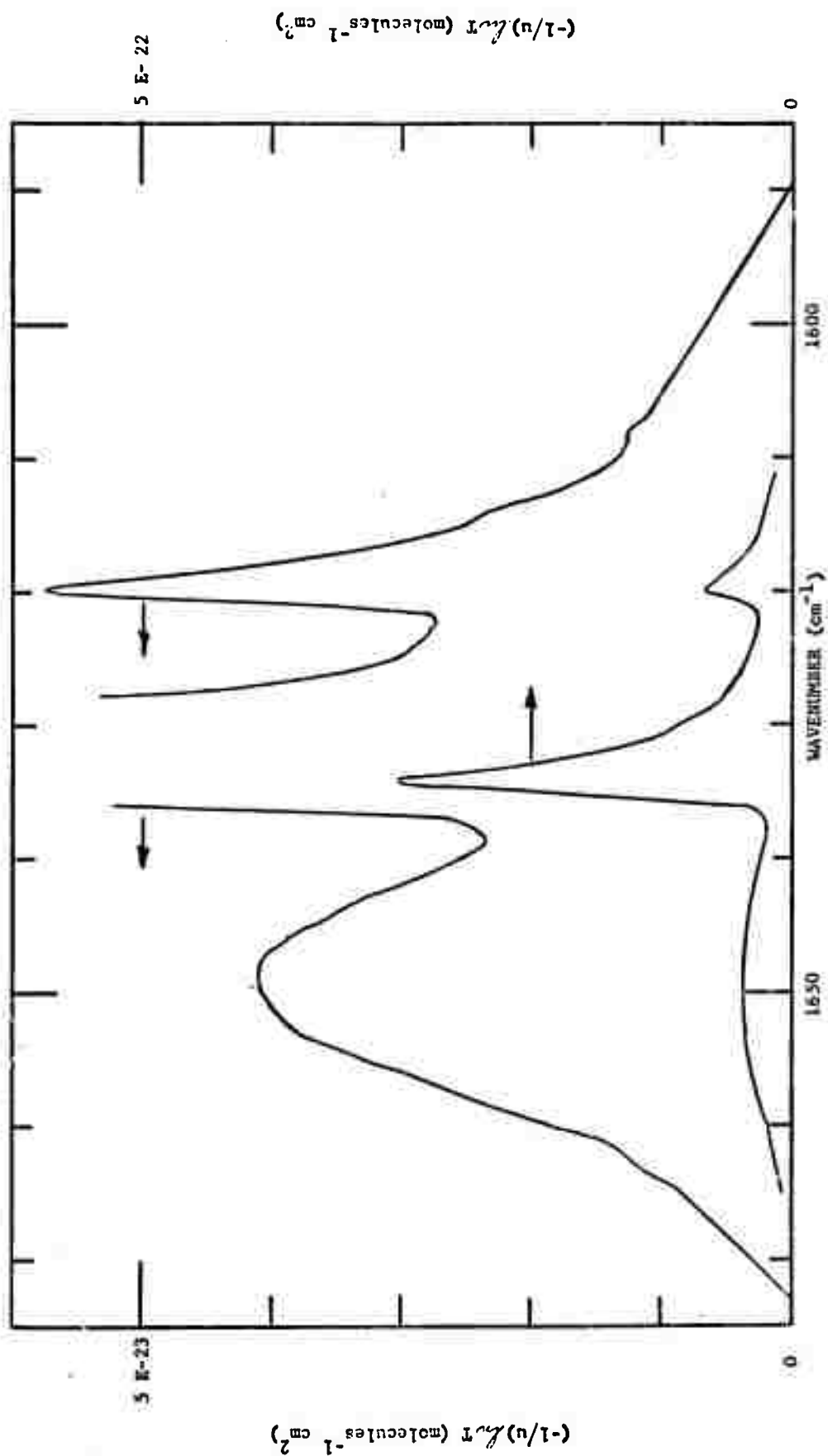


FIG. 3-2. Spectral curve of $(-1/\nu)\Delta T$ from 1595 to 1675 cm^{-1} for an $\text{N}_2\text{O} + \text{N}_2$ sample at 8 atm. $\theta = 290\text{K}$. Spectral slitwidth $\approx 0.5 \text{ cm}^{-1}$. The arrows indicate the ordinate scale to be used.

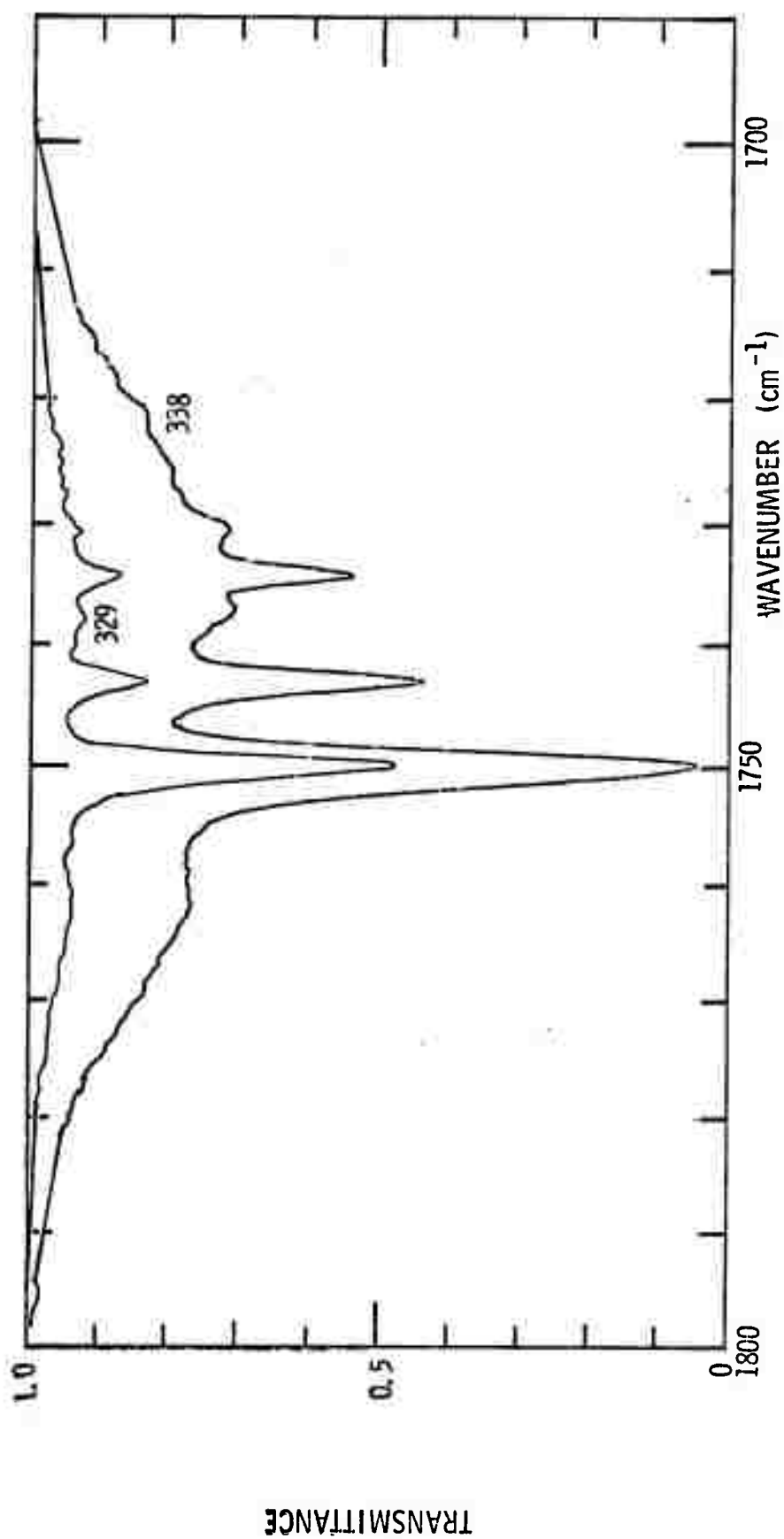


FIG. 3-3. Spectral curves of transmittance from 1690 to 1800 cm^{-1} .

Sample No.	p	P	L	U
	atm	atm	cm	molecules/ cm^2
338	1.0	8.0	416	$103.7 \text{ E } 20$
329	0.197	8.0	416	$20.4 \text{ E } 20$

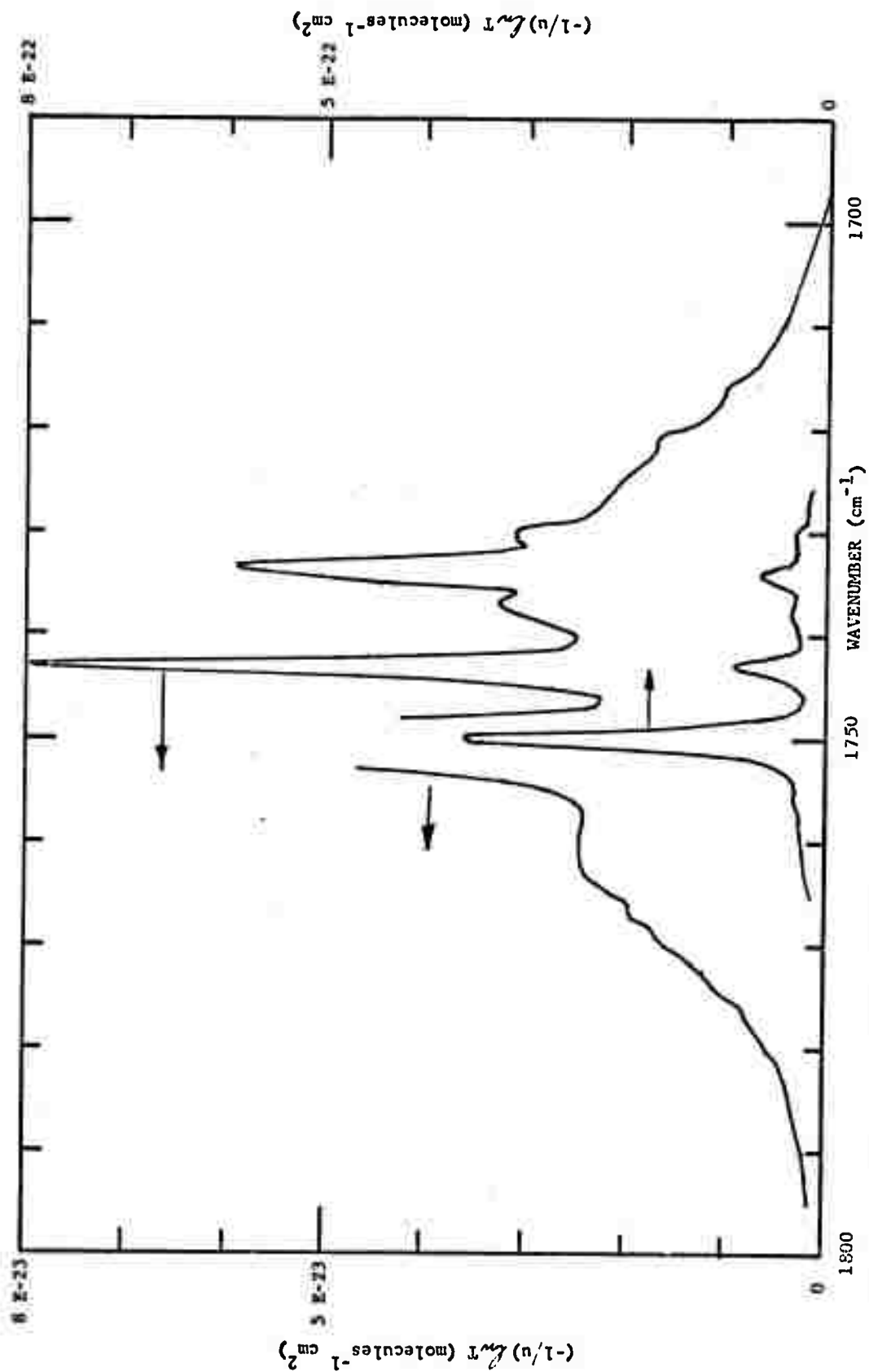


FIG. 3-4. Spectral curve of $(-1/u) dT$ from 1680 to 1800 cm^{-1} for an $\text{N}_2\text{O} + \text{N}_2$ sample at 8 atm. $\theta = 296\text{K}$. Spectral slitwidth $\approx 0.5 \text{ cm}^{-1}$. The arrows indicate the ordinate scale to be used.

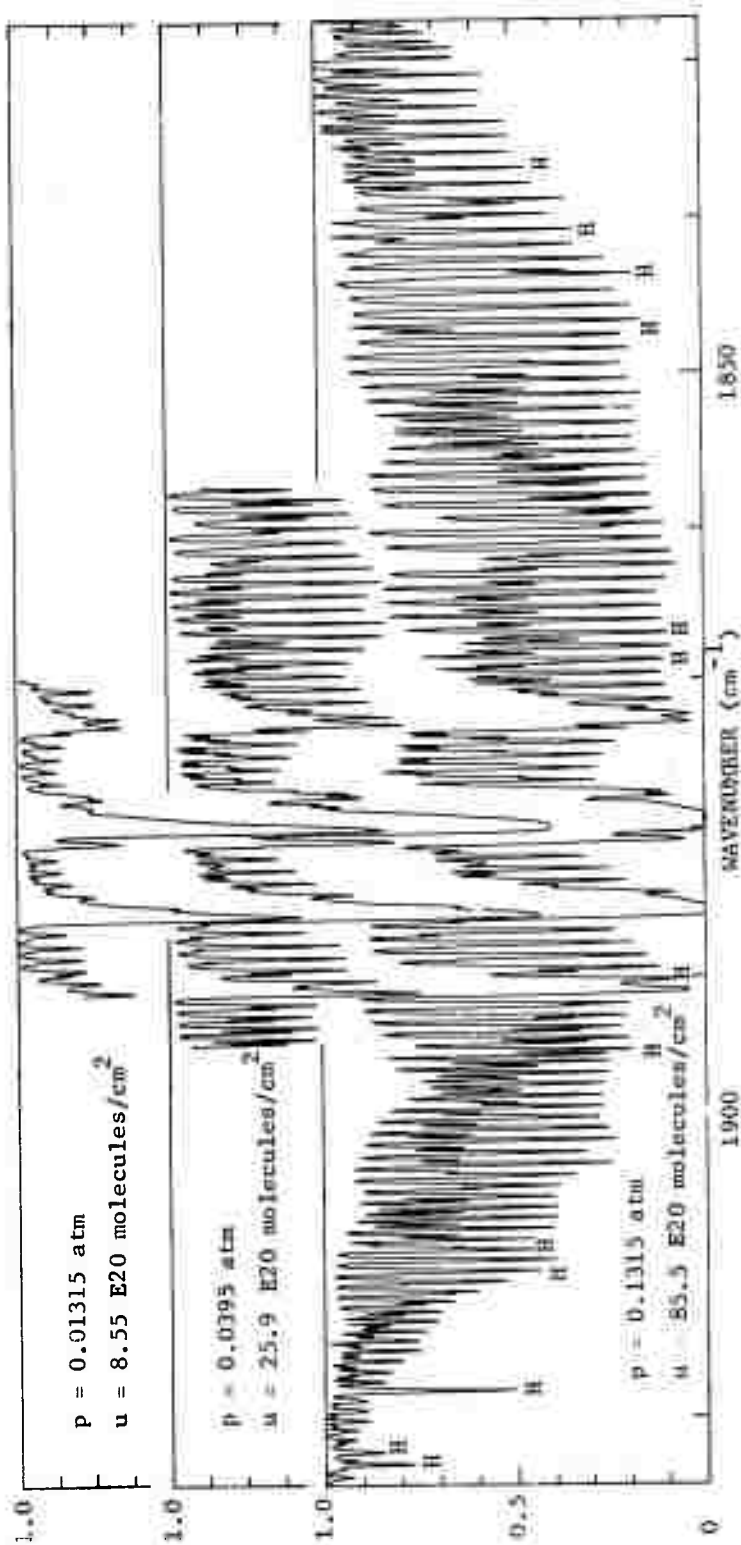
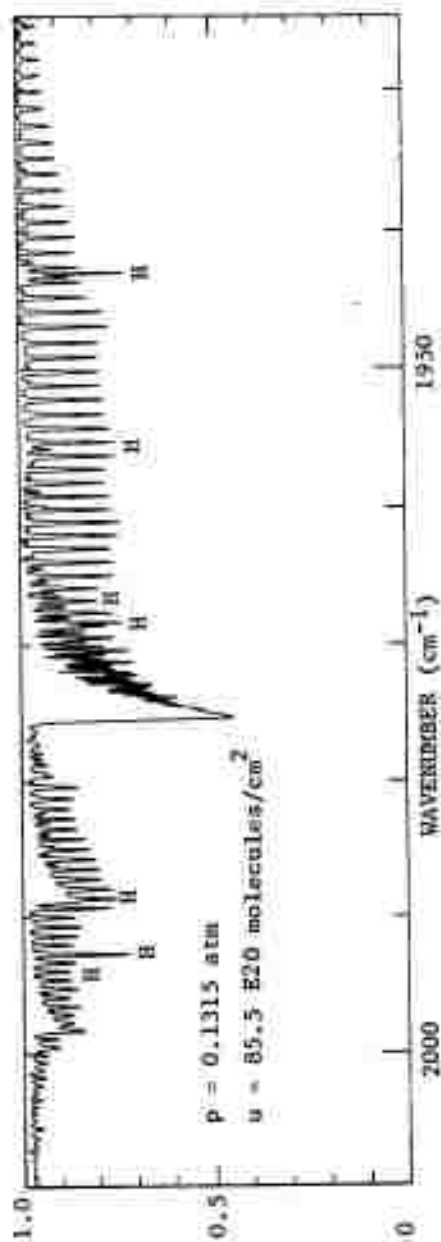
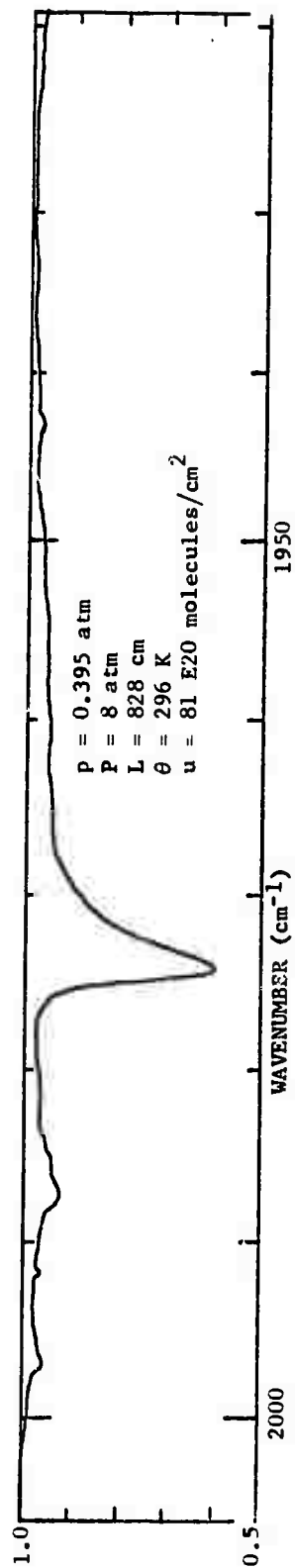


FIG. 3-5. Spectral curves of transmittance between 2010 and 1830 cm^{-1} . All the samples were pure H_2O at 368 K with a path length of 3291 cm^{-1} . The lines marked H are enhanced by H_2O absorption. The lower panel includes two additional curves for smaller samples, the transmittance scales have been displaced. Spectral slitwidth $\approx 0.12 \text{ cm}^{-1}$.



3-9

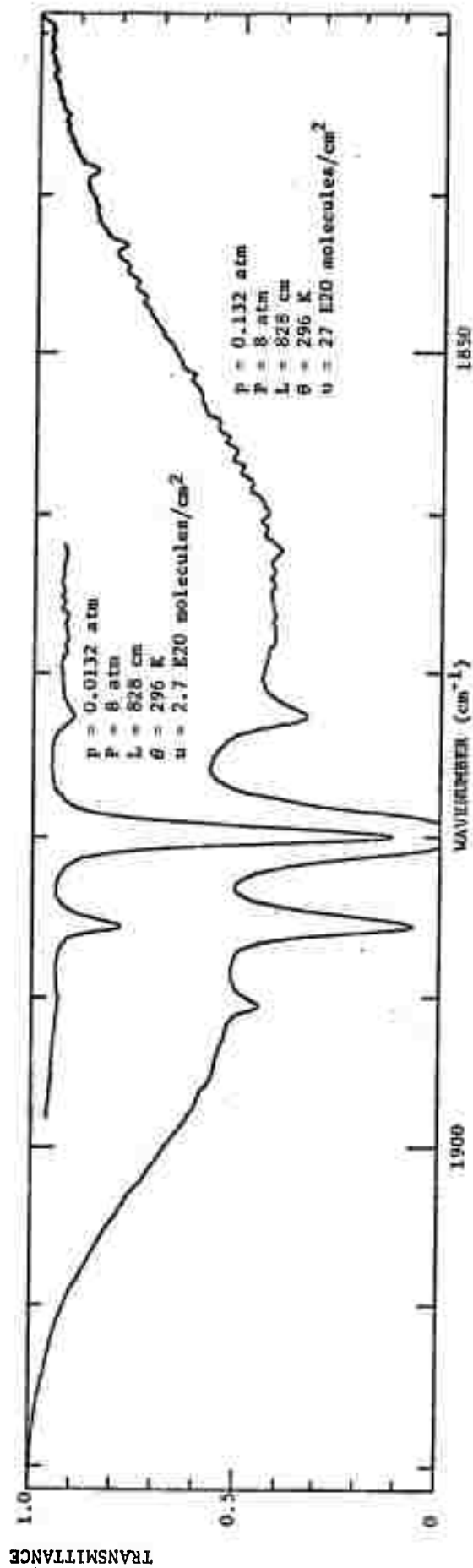


FIG. 3-6. Spectral curves of transmittance from 2005 to 1830 cm^{-1} for N_2O samples pressurized to 8 atm with N_2 . The sample parameters are listed on the figure. The spectral slitwidth $\approx 0.16 \text{ cm}^{-1}$.

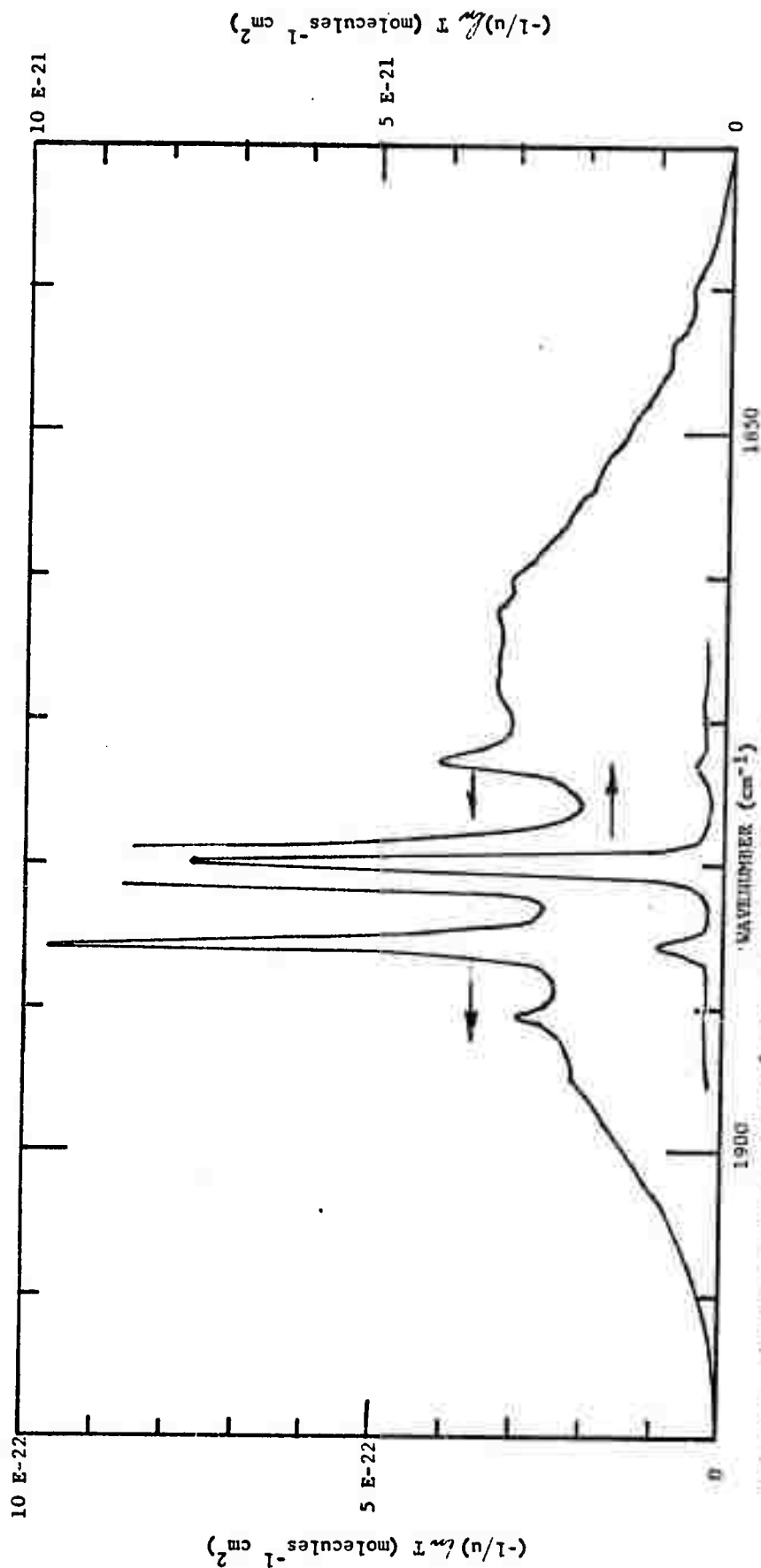


FIG. 3-7. Spectral curve of $(-1/\nu) \frac{dI}{d\nu}$ from 1850 to 1920 cm^{-1} for an $\text{N}_2\text{O} + \text{N}_2$ sample at 0 atm. $\theta = 296\text{K}$. Spectral slitwidth = 0.16 cm^{-1} . The arrows indicate the ordinate scale to be used.

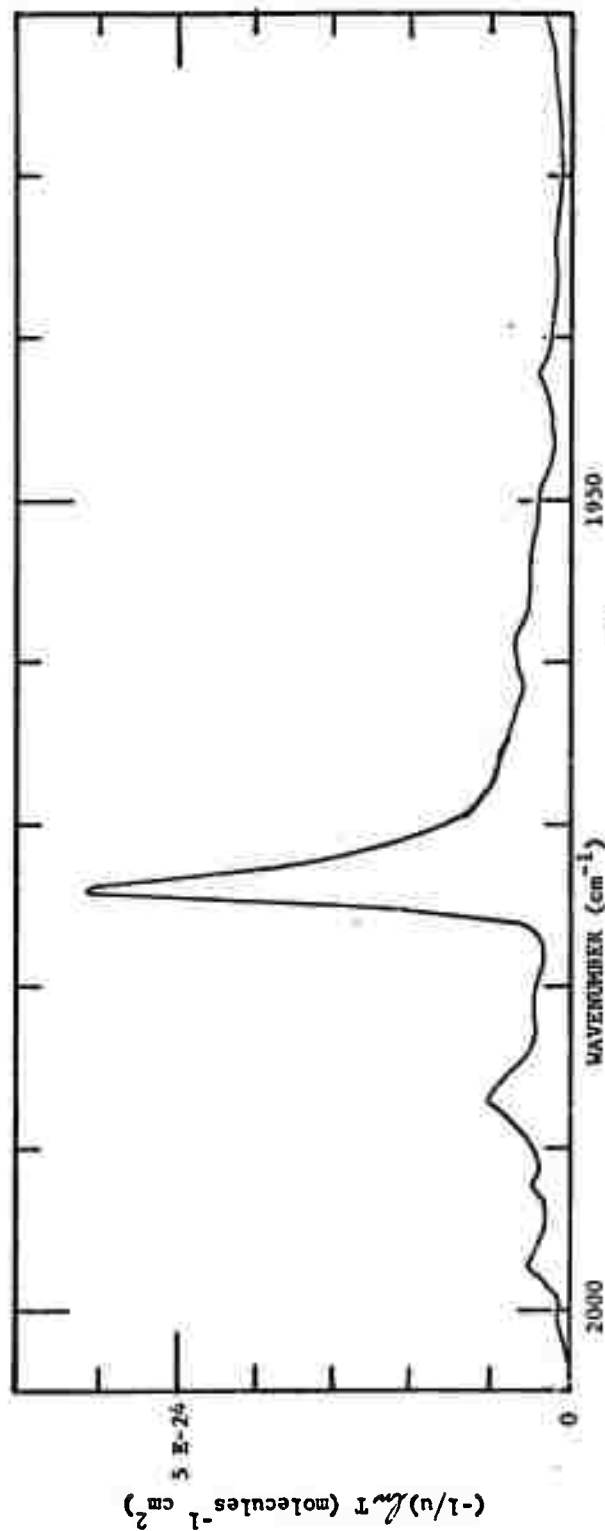


FIG. 3-8. Spectral curve of $(-1/\nu) \frac{dT}{d\nu}$ from 1920 to 2005 cm⁻¹ for an N₂O + N₂ sample at 8 atm. $\theta = 295K$. Spectral slitwidth ± 0.16 cm⁻¹.

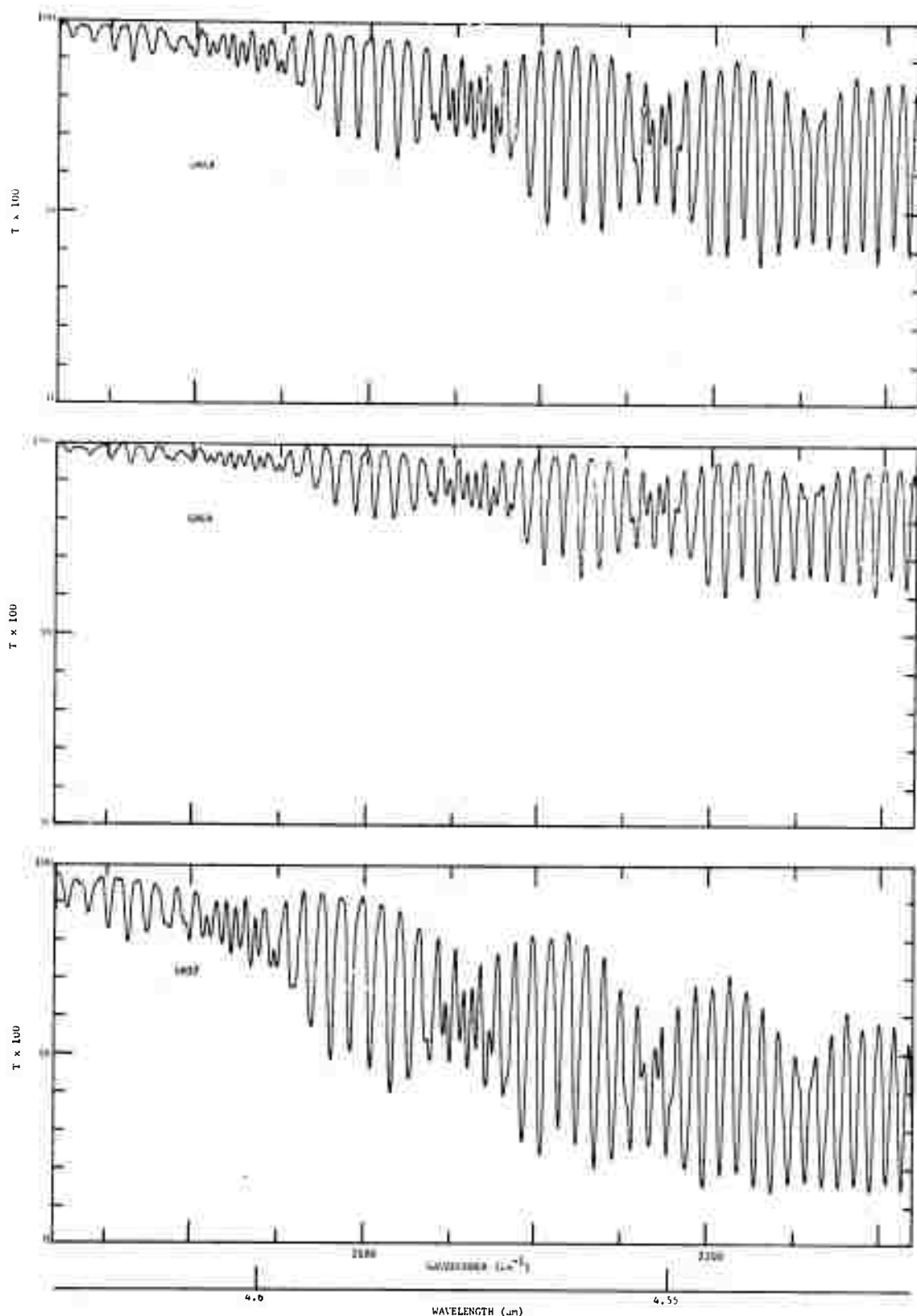


FIG. 3-9. Spectral curves of transmittance between 2165 and 2210 cm^{-1} . The sample parameters are given in Fig. 3-11. Spectral slitwidth $\approx 0.3\text{ cm}^{-1}$.

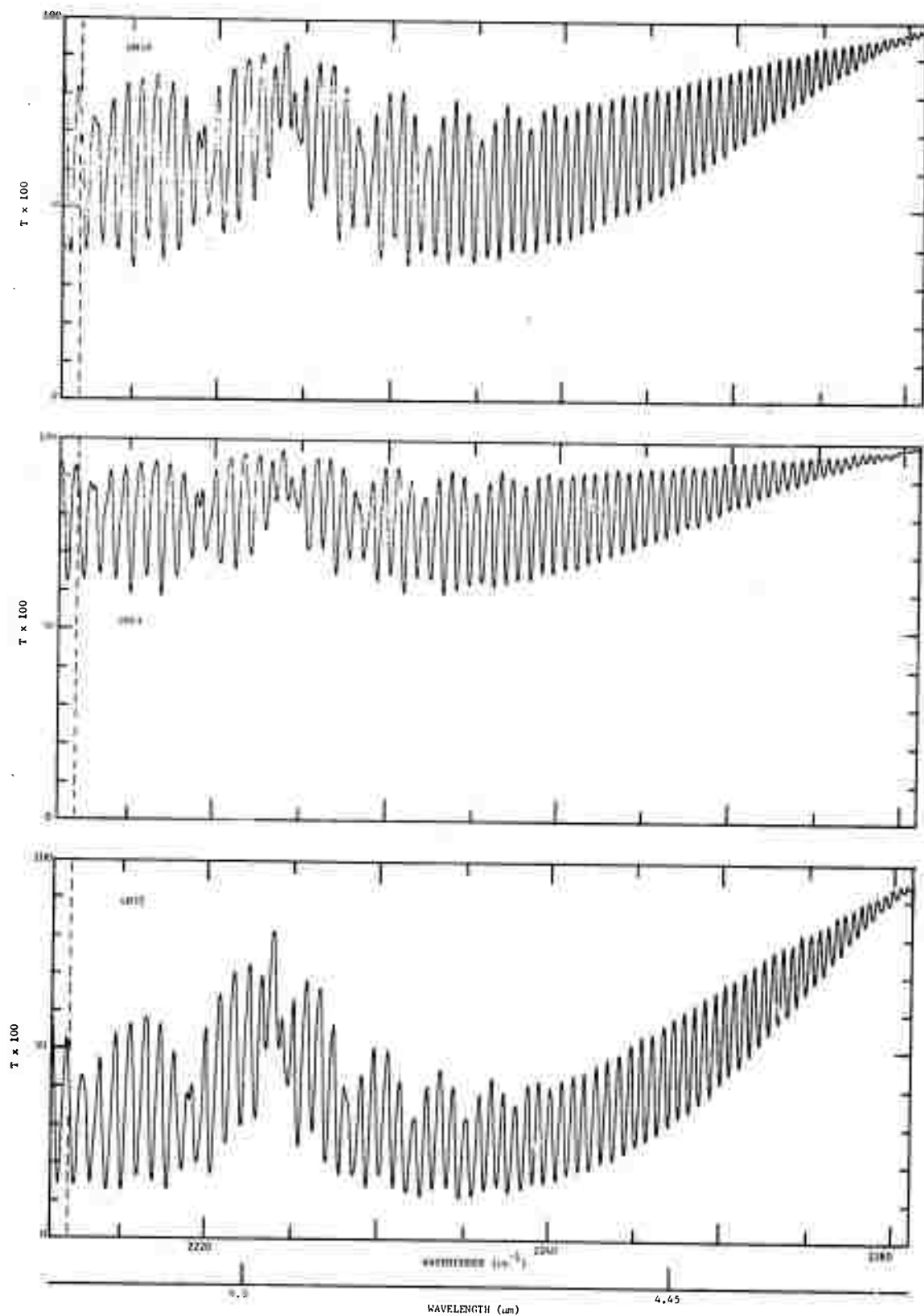
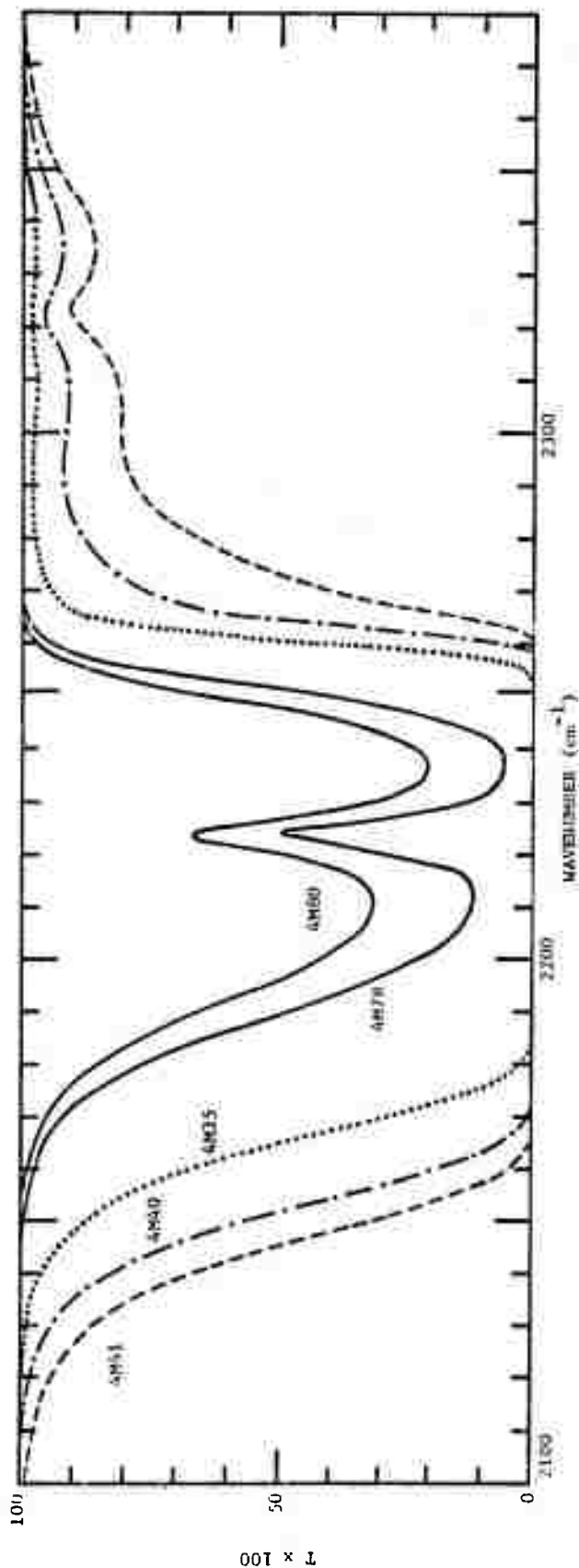


FIG. 3-10. Spectral curves of transmittance between 2210 and 2260 cm^{-1} . The sample parameters are given in Fig. 3-11. Spectral slitwidth $\approx 0.3\text{ cm}^{-1}$.



Sample Number	P atm	P _{N₂} atm	P atm	u molecules/cm ²	Temperature °K	L Meters
4M35	13.59	11.55	2.04	30.1	302	0.00602
4M40	7.80	0	7.80	118.6	302	0.00602
4M41	13.59	0	13.59	212.3	302	0.00602
4M48	0.1250	0	0.1250	1.845	300	0.00602
4M49	0.0625	0	0.0625	0.922	300	0.00602
4M57	0.257	0	0.257	3.77	301	0.00602
4M78	8.03	7.23	0.803	2.00	301	0.00102
4M80	9.03	8.57	0.453	1.12	302	0.00102

FIG. 3-11. Spectral curves of transmittance from 2100 to 2380 cm^{-1} for several samples at pressures greater than 7 atm. Spectral slitwidth $\approx 0.3 \text{ cm}^{-1}$. The sample parameters for the spectra shown in Figures 3-9, 3-10 and 3-11 are given in the table below the figure.

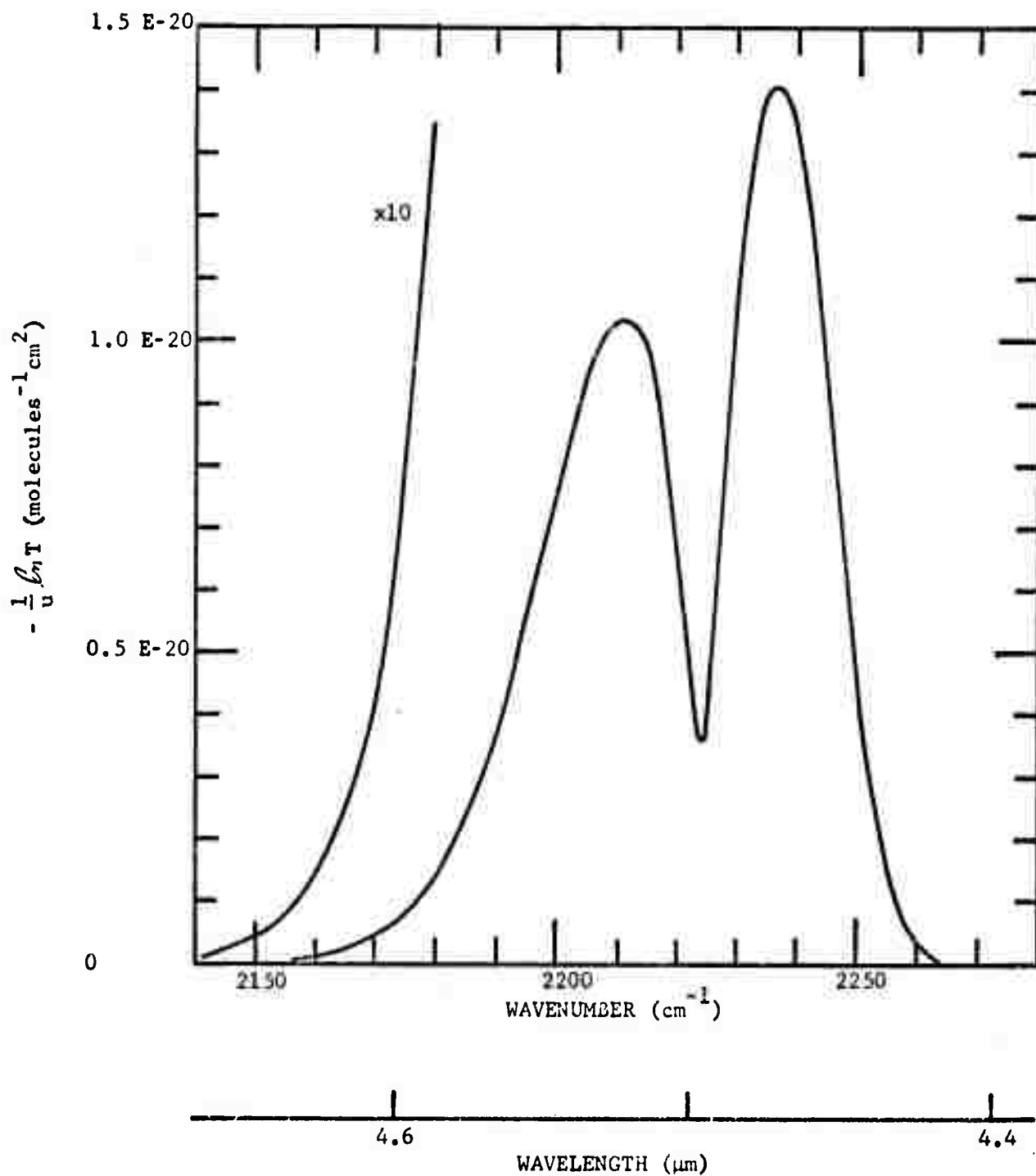


FIG. 3-12. Spectral curves of $(-1/u) \ln T$ between 2140 and 2280 cm^{-1} . The curves are based on transmittance curves such as those in Fig. 3-11 which represent samples at sufficiently high pressure that the line structure is smoothed out. Values were multiplied by 10 before plotting the points for the left-hand curve.

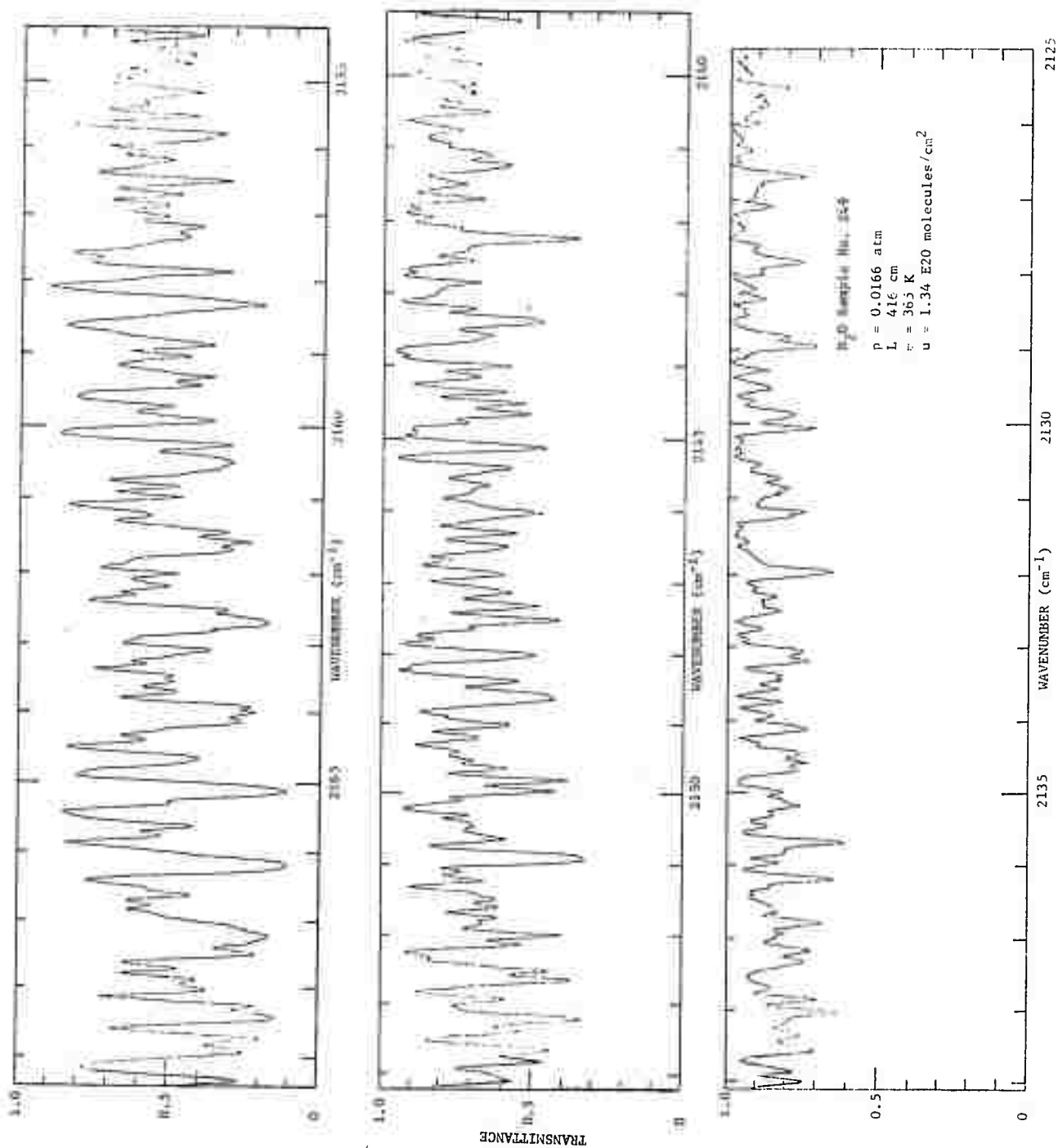


FIG. 3-13. Spectral plot of transmittance from 2125 to 2169 cm^{-1} for a pure sample of N_2O at 365 K. The sample parameters are listed in one of the panels. The spectral slitwidth $\approx 0.07 \text{ cm}^{-1}$.

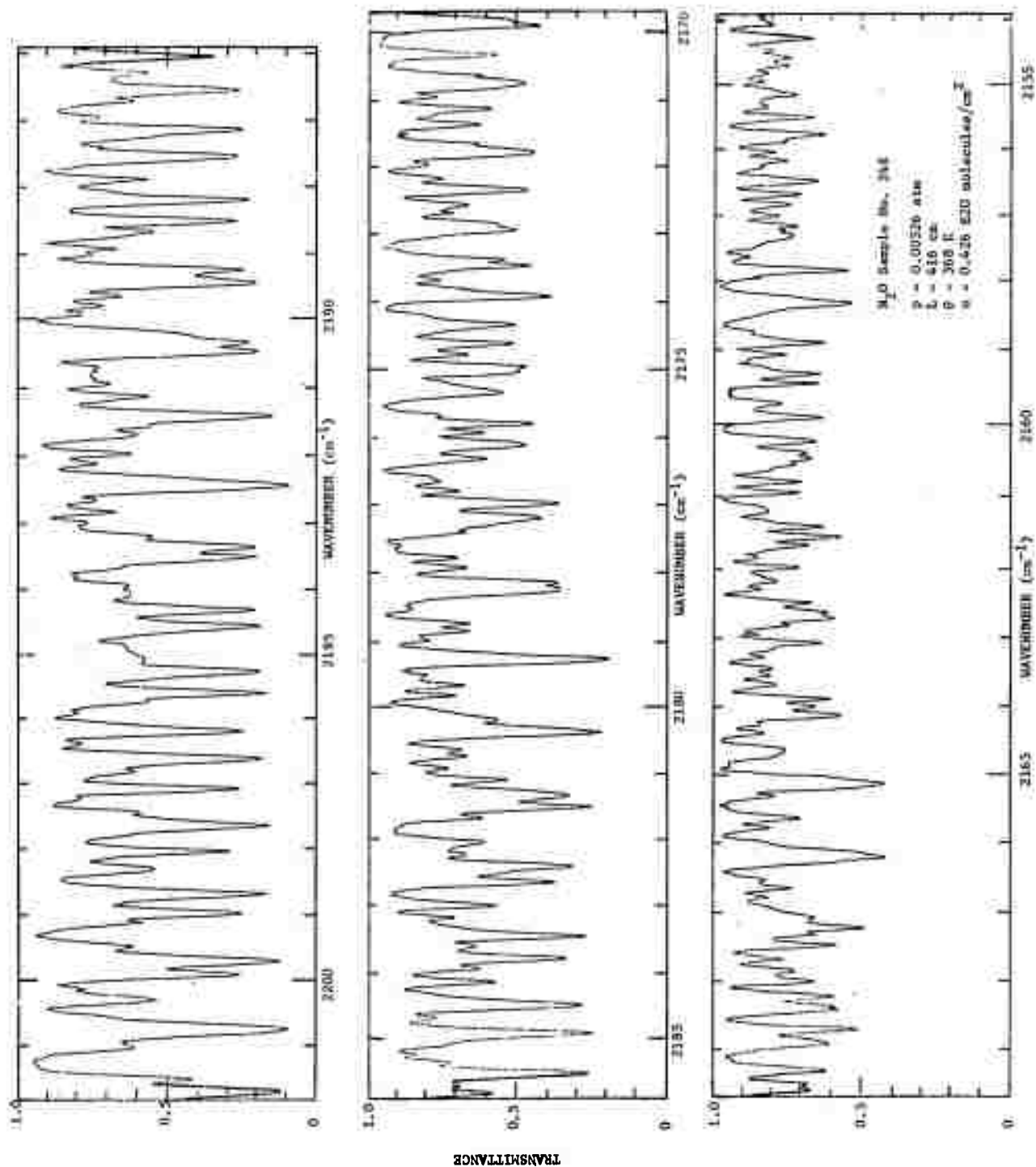


FIG. 3-14. Spectral plot of transmittance from 2154 to 2202 cm^{-1} for a pure N₂O sample at 368 K. The sample parameters are listed on the bottom panel. Spectral slitwidth ≈ 0.07 cm^{-1} .

for pure samples elevated to 368 K in order to enhance the absorption by the lines of the difference bands and by lines in the wings of the main band so that they could be identified more easily.

2260-2380 cm⁻¹

The primary absorption band ($04^0_0 \leftarrow 00^0_0$) in this region is centered at 2322.624 cm⁻¹. The main features can be seen in Fig. 3-15. A few lines near the center of the main band belong to the $05^1_0 \leftarrow 01^1_0$ band. There was no evidence of the $10^0_1 \leftarrow 02^0_0$ band whose center would be at 2312.687 cm⁻¹.

Figure 3-16 shows spectral plots of transmittance from 2308 to 2327 cm⁻¹ at rather high resolution, 0.11 cm⁻¹. The lines due to the $05^1_0 \leftarrow 01^1_0$ can easily be identified near the center of the main band, 00^0_1 . Also, the Q-branch of the difference band is observable near 2309 cm⁻¹ between the P16 and P17 lines of the main band. The lines of the difference band near the band center of the main band are isolated from the main band and were identified as the R14, R15, and R16 lines of the $05^{1d}_0 \leftarrow 01^{1d}_0$ sub-band and the R15 of the $05^{1c}_0 \leftarrow 01^{1c}_0$ sub-band.

The R15 $05^{1c}_0 \leftarrow 01^{1c}_0$ line was well isolated from the main band so that its intensity could be measured. We found

$$S_J(R15 \ 05^{1c}_0 \leftarrow 01^{1c}_0) = 3.5 \pm 0.4 \times 10^{-23} \text{ molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}.$$

From the results given by Young⁷ we can determine the total band intensity from the line intensity. $S_v(05^1_0 \leftarrow 01^1_0) = 0.34 \pm 0.04 \times 10^{-20} \text{ molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$. This value includes the contribution from the 4 sub-bands $05^{1c}_0 \leftarrow 01^{1c}_0$, $05^{1d}_0 \leftarrow 01^{1d}_0$, $05^{1c}_0 \leftarrow 01^{1d}_0$ and $05^{1d}_0 \leftarrow 01^{1c}_0$.

The line positions for the 04^0_0 band were calculated using Pliva's¹⁰ rotational constants and were compared to the observed line positions that were determined with the use of known positions of nearby CO₂ lines. The calculated positions of the R35 to R40 lines of N₂O deviated by as much as 0.15 cm⁻¹ from the observed and the P1 line by approximately 0.08 cm⁻¹. We have redetermined the rotational constants and band center for the 04^0_0 and $05^1_0 \leftarrow 01^1_0$ bands and listed them in Tables 2-1 and 2-2. The letter "C" in Fig. 3-16 indicates positions of CO₂ lines that may contribute to the absorption since they are so intense that a trace of CO₂ impurity in the sample, or elsewhere in the optical path, can cause significant absorption. As an example, the weak line near 2317.2 cm⁻¹ is the P36 line of CO₂.

2400-2630 cm⁻¹

The strong absorption bands, $20^0_0 \leftarrow 00^0_0$ and the $12^0_0 \leftarrow 00^0_0$, are centered at 2563.341 and 2461.998 cm⁻¹, respectively. Figure 3-17 shows transmittance

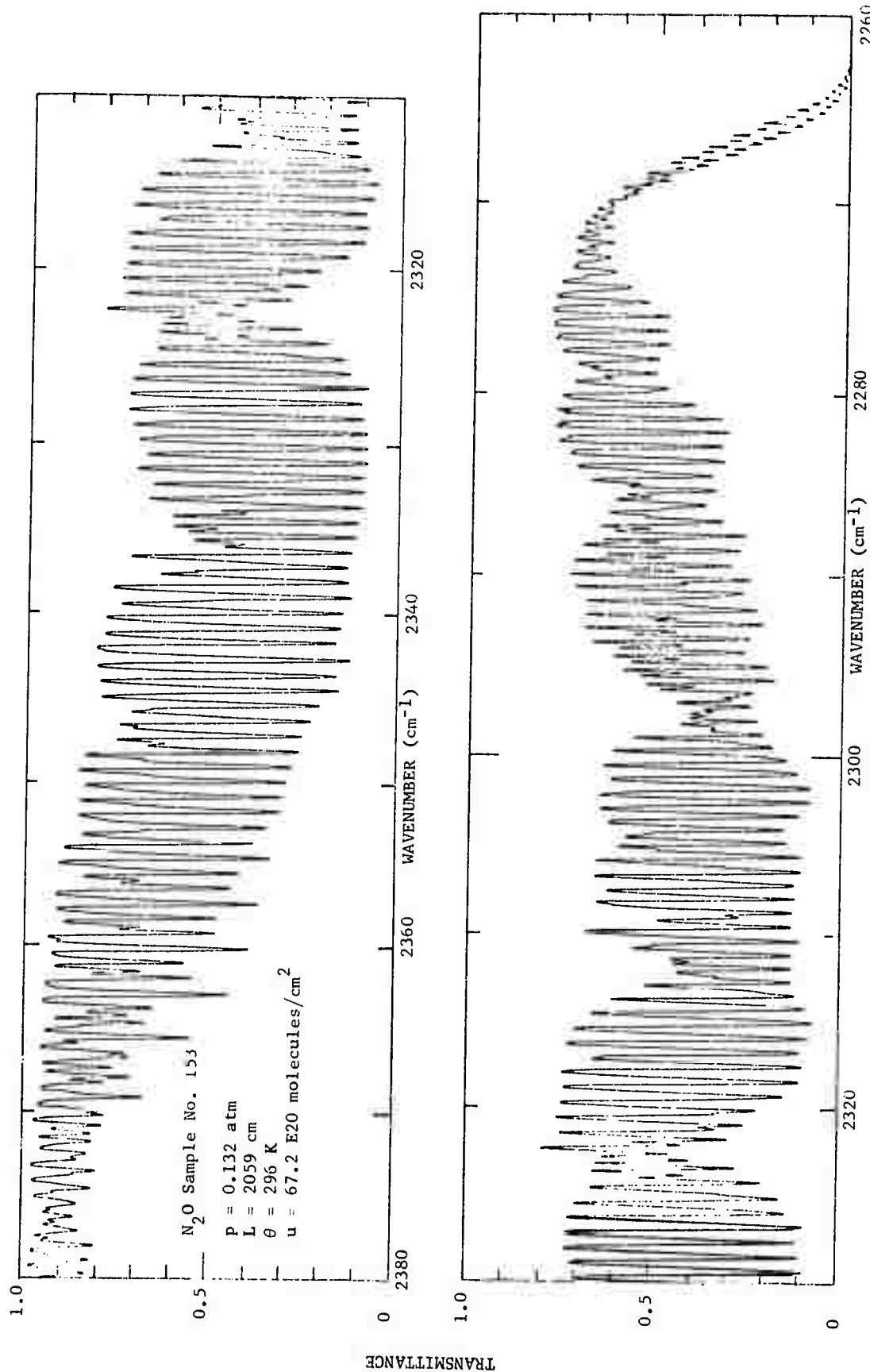


FIG. 3-15. Spectral plot of transmittance between 2260 and 2380 cm⁻¹ for a pure N₂O sample. The sample parameters are listed in the top panel. Spectral slitwidth ≈ 0.18 cm⁻¹.

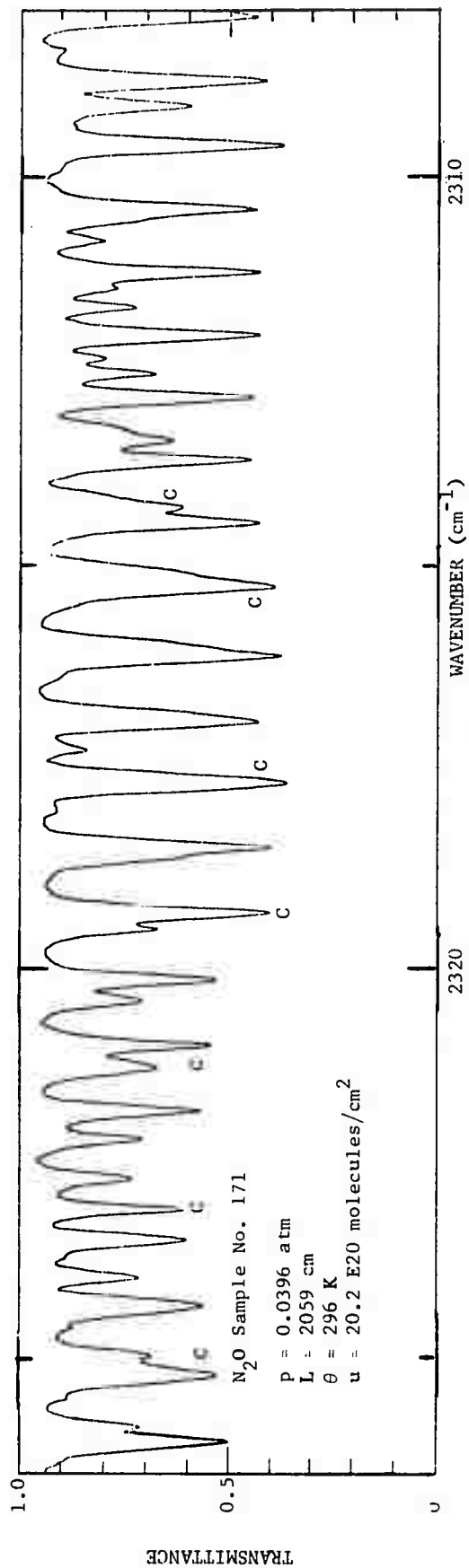
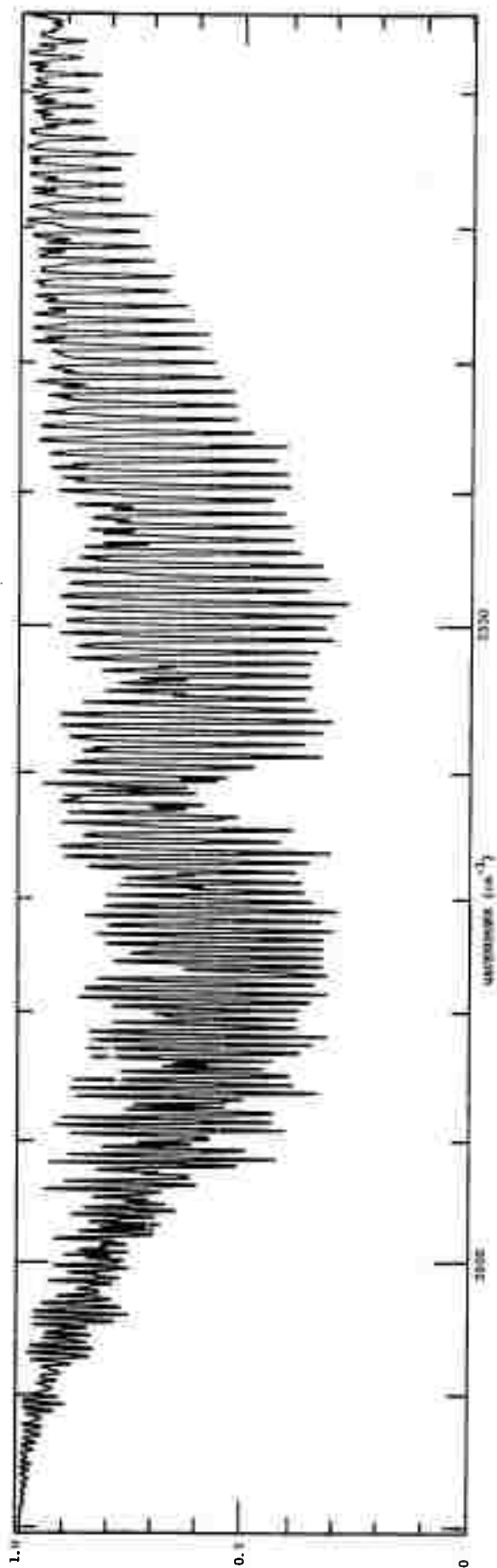


FIG. 3-16. Spectral plot of transmittance from 2308 to 2327 cm^{-1} for a pure sample of N_2O . The sample parameters are listed in the panel. Spectral slitwidth $\approx 0.11 \text{ cm}^{-1}$. The letter C indicates the positions of CO_2 lines that may be absorbing appreciably.



TRANSMITTANCE

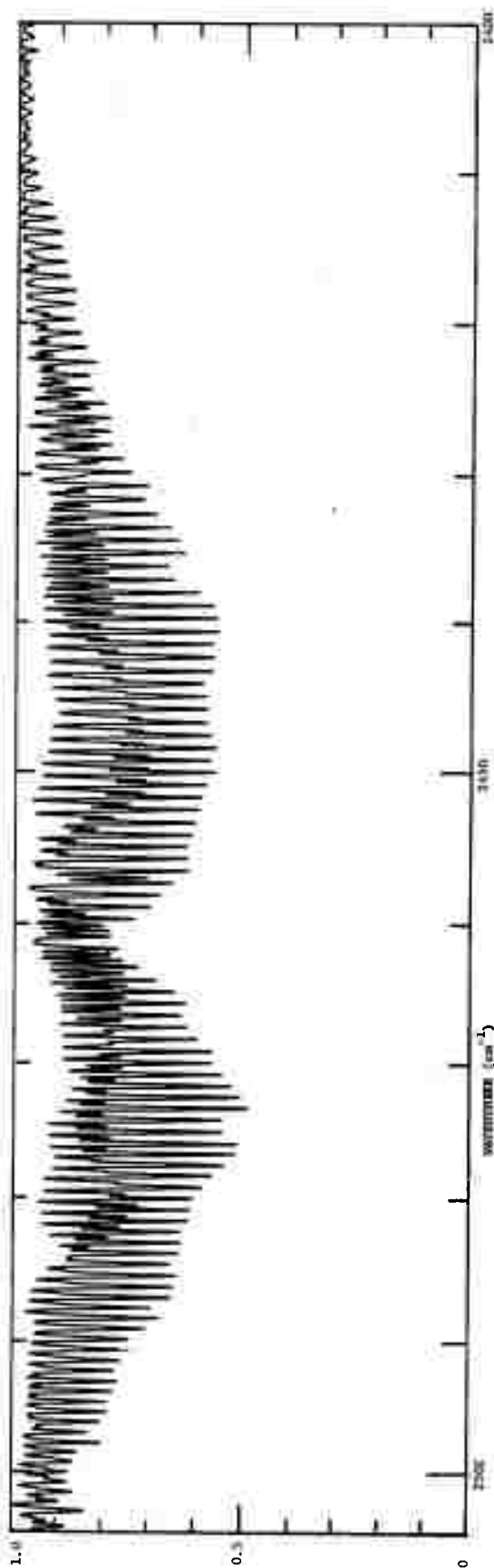


FIG. 3-17. Spectral curve of transmittance from 2400 to 2620 cm^{-1} for a pure sample of N_2O , $p = 0.0263 \text{ atm}$, $L = 416 \text{ cm}$, $\theta = 296 \text{ K}$, and $u = 2.71 \times 10^{20} \text{ molecules/cm}^2$. Spectral slitwidth $= 0.11 \text{ cm}^{-1}$.

curves of both of these band systems for a pure sample of N_2O at relatively high resolution. Each of these band systems contain several difference bands that contribute significantly to the features seen in the spectrum. In the $12^{00}0 \leftarrow 00^{00}0$ band system, we have identified lines of the $13^{10}0 \leftarrow 01^{10}0$, $14^{00}0 \leftarrow 02^{00}0$ and $14^{20}0 \leftarrow 02^{20}0$ bands. The $20^{00}0 \leftarrow 00^{00}0$ band system contains the following observable bands: $21^{10}0 \leftarrow 01^{10}0$, $22^{00}0 \leftarrow 02^{00}0$, $22^{20}0 \leftarrow 02^{20}0$ and $30^{00}0 \leftarrow 10^{00}0$. The ℓ -type doubling of the lines was observed in the $13^{10}0 \leftarrow 01^{10}0$ and $21^{10}0 \leftarrow 01^{10}0$ bands.

Figure 3-18 shows a transmittance curve for a pure sample of N_2O between 2432 and 2440 cm^{-1} . The lines are identified by the solid and dashed lines. The strong lines are P27 through P34 of the main band ($12^{00}0 \leftarrow 00^{00}0$). The weaker lines are P20 through P29 of the $13^{10}0 \leftarrow 01^{10}0$ sub-band. The P21 through P29 lines arising from the $01^{1d}0$ energy level are not evident in this region since they are nearly coincident with the lines of the main band.

The contour of the envelope of the maximum absorptance of the $12^{00}0 \leftarrow 00^{00}0$ lines has a dip at lines P29 and P30. This is probably due to the close coincidence of the P29 and P30 lines of the main band with the P24 and P25 lines of the $13^{1d}0 \leftarrow 01^{1d}0$ sub-band. The rest of the lines of these two bands are separated more. However, in calculating line positions using the rotational constants of Pliva¹⁰ the coincidence occurs at line P27 and P28 of the main band instead of the P29 and P30 lines. The calculated line positions are given in the table below. It seems probable that Pliva's constants contain significant error but were not changed in the parameter table. Further investigation of this is in order.

TABLE 3-1

CALCULATED LINE POSITIONS

	$12^{00}0 \leftarrow 00^{00}0$ cm^{-1}		$13^{1d}0 \leftarrow 01^{1d}0$ cm^{-1}	$\Delta\nu_{0,1}$ cm^{-1}
P26	2439.633	P21	2439.593	0.040
P27	38.747	P22	38.729	0.018
P28	37.858	P23	37.864	0.006
P29	36.968	P24	36.998	0.030
P30	36.075	P25	36.131	0.056
P31	35.180	P26	35.262	0.082

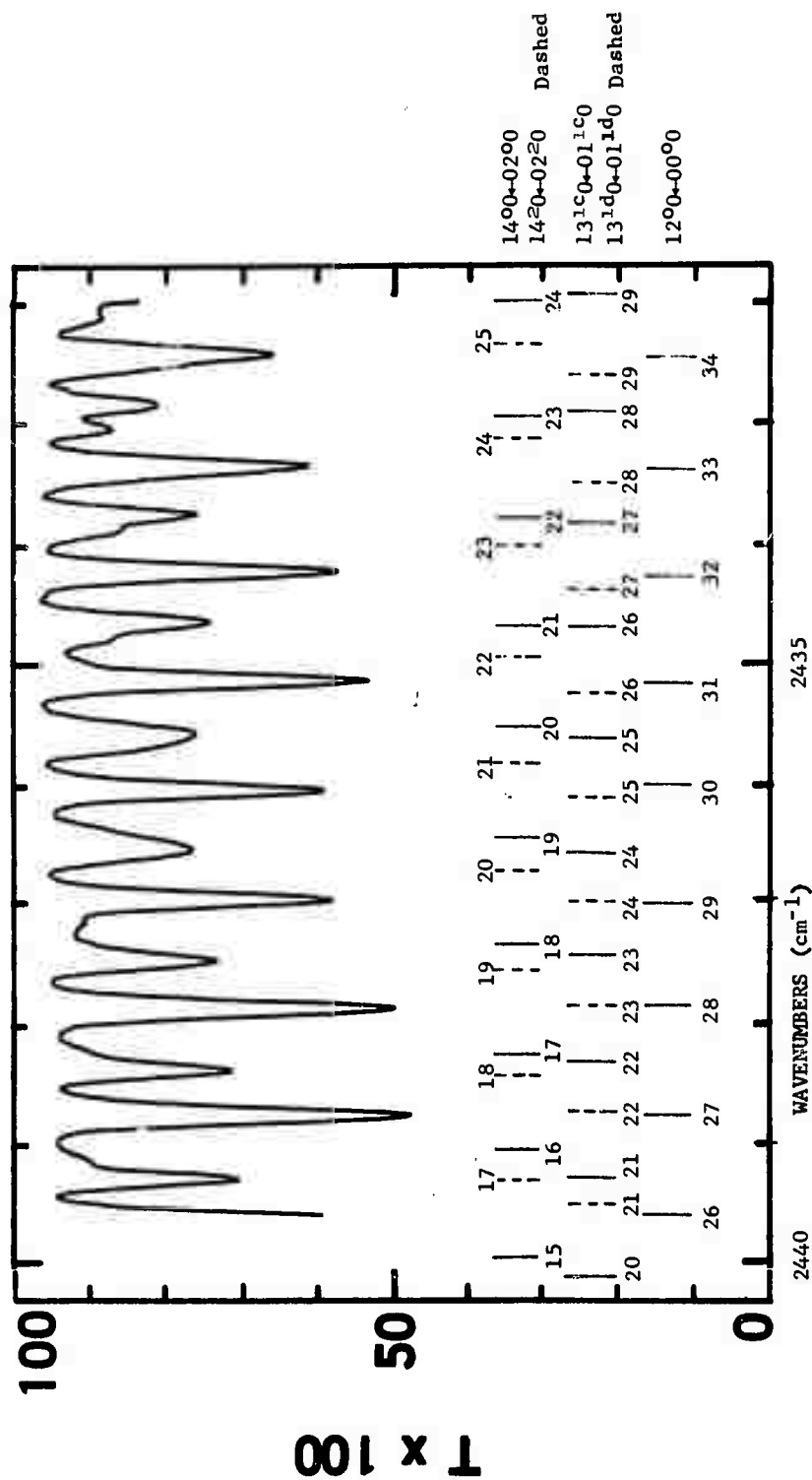


FIG. 3-18. Spectral curve of transmittance from 2432 to 2440 cm^{-1} for a pure sample of N_2O ; $p = 0.0101$ atm, $L = 1648$ cm, $\theta = 296K$ and $u = 4.14 \times 10^{20}$ molecules/ cm^2 . The calculated positions of the lines due to the $12^{00}-00^{00}$, $13^{10}-01^{10}$, $13^{10}-01^{10}$, $14^{00}-02^{00}$ and $14^{20}-02^{20}$ transitions are indicated. The L -type splitting of the $14^{20}-02^{20}$ transitions is not appreciable at these J values.

Figures 3-19 and 3-20 show curves of transmittance and $(-1/u) \ln T$ for $N_2O + N_2$ samples at approximately 6 atm pressure. There was some structure in the original transmittance curves that was smoothed out before replotting the curve. The intensity of the $12^{00}-00^{00}$ band system, $33.4 \times 10^{-20} \pm 5\%$ molecules $^{-1}$ cm 2 cm $^{-1}$, is less than the values 42.8×10^{-20} and 37.6×10^{-20} molecules $^{-1}$ cm 2 cm $^{-1}$ reported by Burch and Williams¹³ and by Vincent-Geisse,¹⁴ respectively. The intensity of the $20^{00}-00^{00}$ band system is $135 \times 10^{-20} \pm 5\%$ molecules $^{-1}$ cm 2 cm $^{-1}$, which compares well with 132×10^{-20} molecules $^{-1}$ cm 2 cm $^{-1}$ reported by Vincent-Geisse. Burch and Williams reported a larger value, 163×10^{-20} molecules $^{-1}$ cm 2 cm $^{-1}$. In view of improved experimental methods, we feel that the values found in the present investigation are most reliable.

2630-2840 cm $^{-1}$

The main absorption band (01^11-00^00) is centered at 2798.290 cm $^{-1}$. We also observed a weaker band not shown in any of the figures in this report and identified it as the $30^{00}-02^00$ band centered at 2668.24 cm $^{-1}$. Its intensity is approximately 0.003×10^{-20} molecules $^{-1}$ cm 2 cm $^{-1}$. We also looked for evidence of the 03^10-10^00 band, whose center would occur at 2646.35 cm $^{-1}$ but could find none in the spectrum of a sample of 1 atm of pure N_2O with a path length of 20 meters.

The main absorption features between 2725 and 2840 cm $^{-1}$ are due to the 01^11-00^00 band and its associated hot bands, 02^01-01^10 and 02^20-01^10 , centered at 2798.290 , 2775.207 and 2784.370 cm $^{-1}$, respectively. The Q-branches of the three bands are apparent in Figs. 3-21 and 3-22. Tidwell, Flyler and Benedict¹⁵ identified these bands as well as the 11^11-10^00 , 03^31-02^20 , 03^11-02^00 , and 03^11-02^20 bands at 2776.06 , 2770.39 , 2763.124 and 2753.518 cm $^{-1}$, respectively. They also identified bands of some of the rarer isotopes such as the 01^11-00^00 bands of $^{14}N^{14}N^{18}O$ centered at 2787.2 cm $^{-1}$ and the 02^21-01^10 and 01^11-00^00 band of $^{14}N^{15}N^{16}O$ centered at 2726.5 and 2739.6 cm $^{-1}$, respectively.

The intensities of the Q-branches were measured from plots of $(-1/u) \ln T$ by determining what portions of the curves were due to the P- and R-branches, and what portions were due to the Q-branch. The intensities with $\pm 5\%$ uncertainty were found to be in molecules $^{-1}$ cm 2 cm $^{-1}$:

$$\begin{aligned} S_Q(01^11) &= 3.17 \times 10^{-20} \\ S_Q(02^21) &= 0.391 \times 10^{-20} \\ S_Q(02^01) &= 0.171 \times 10^{-20} \end{aligned}$$

The intensities of the Q-branches are in the expected proportion based on simple theory.

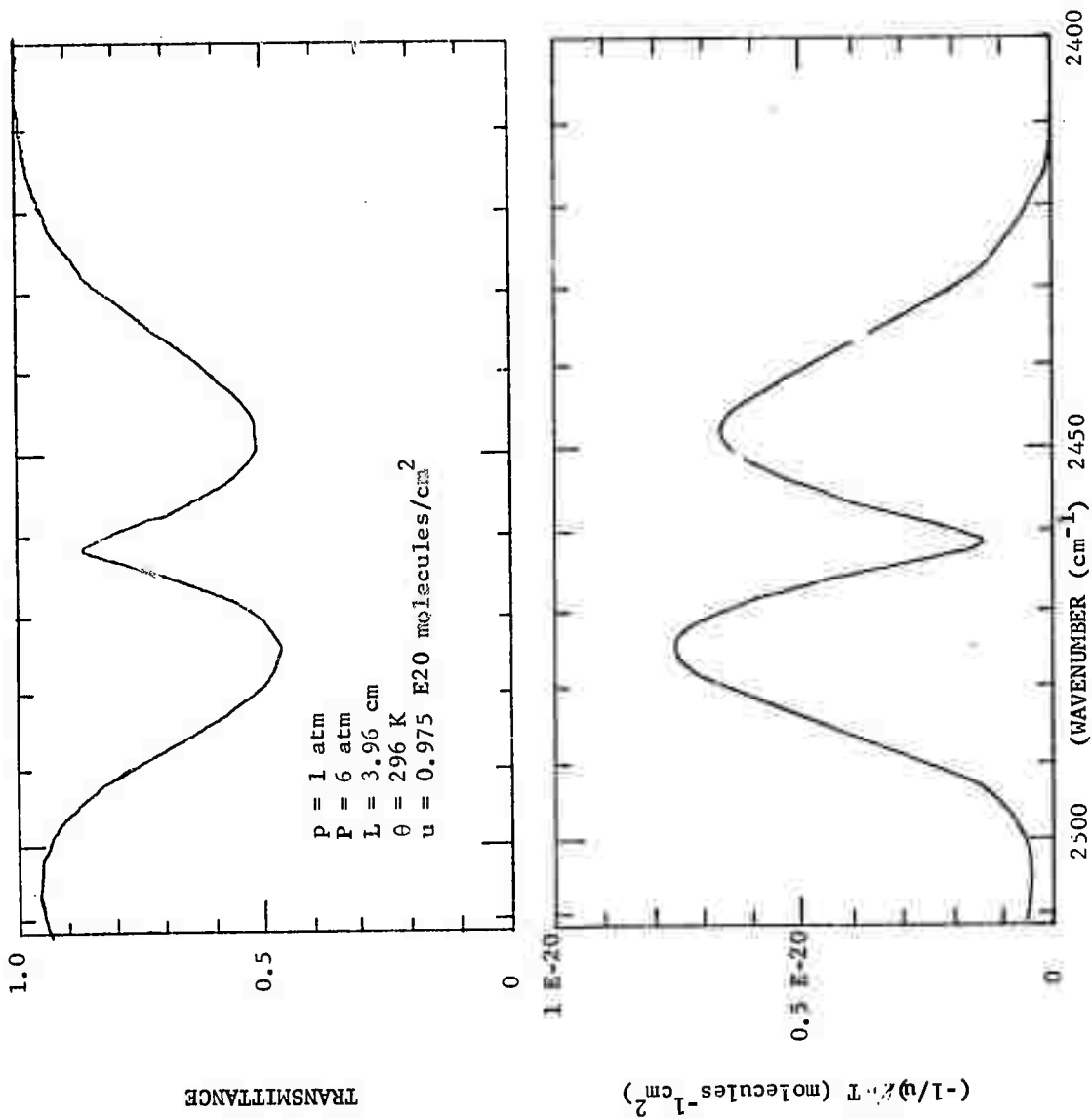


FIG. 3-19. Spectral curves of transmittance and $(-1/u) \ln T$ from 2400 to 2510 cm^{-1} . The sample parameters for the transmittance curve are listed in the upper panel. p denotes the partial pressure of N_2O and P denotes the total pressure $\text{N}_2\text{O} + \text{N}_2$.

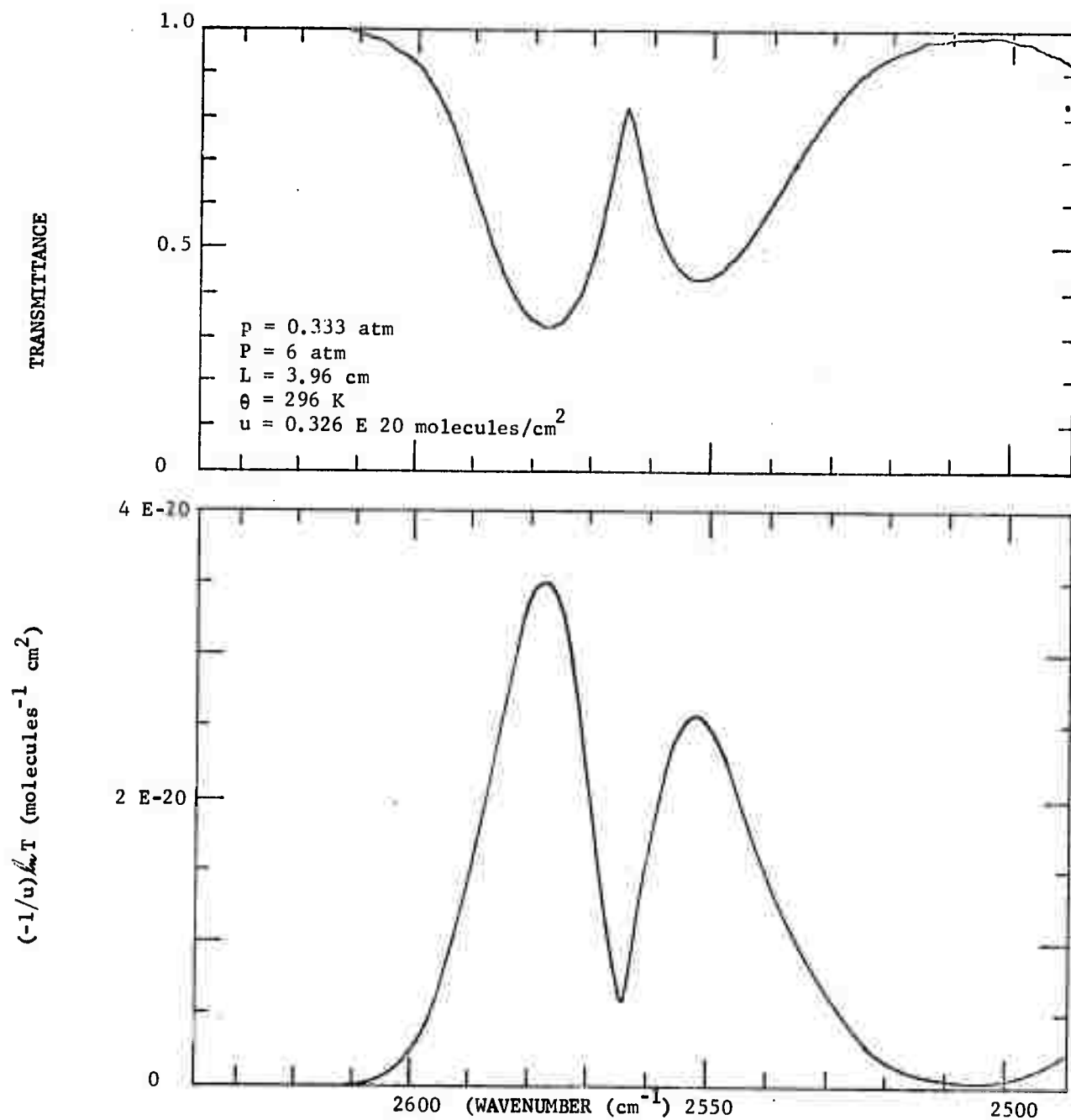


FIG. 3-20. Spectral curves of transmittance and $(-1/u) \ln T$ from 2490 to 2640 cm^{-1} . The sample parameters for the transmittance curve are listed in the upper panel. p denotes the partial pressure of N_2O and P denotes the total pressure $\text{N}_2\text{O} + \text{N}_2$.

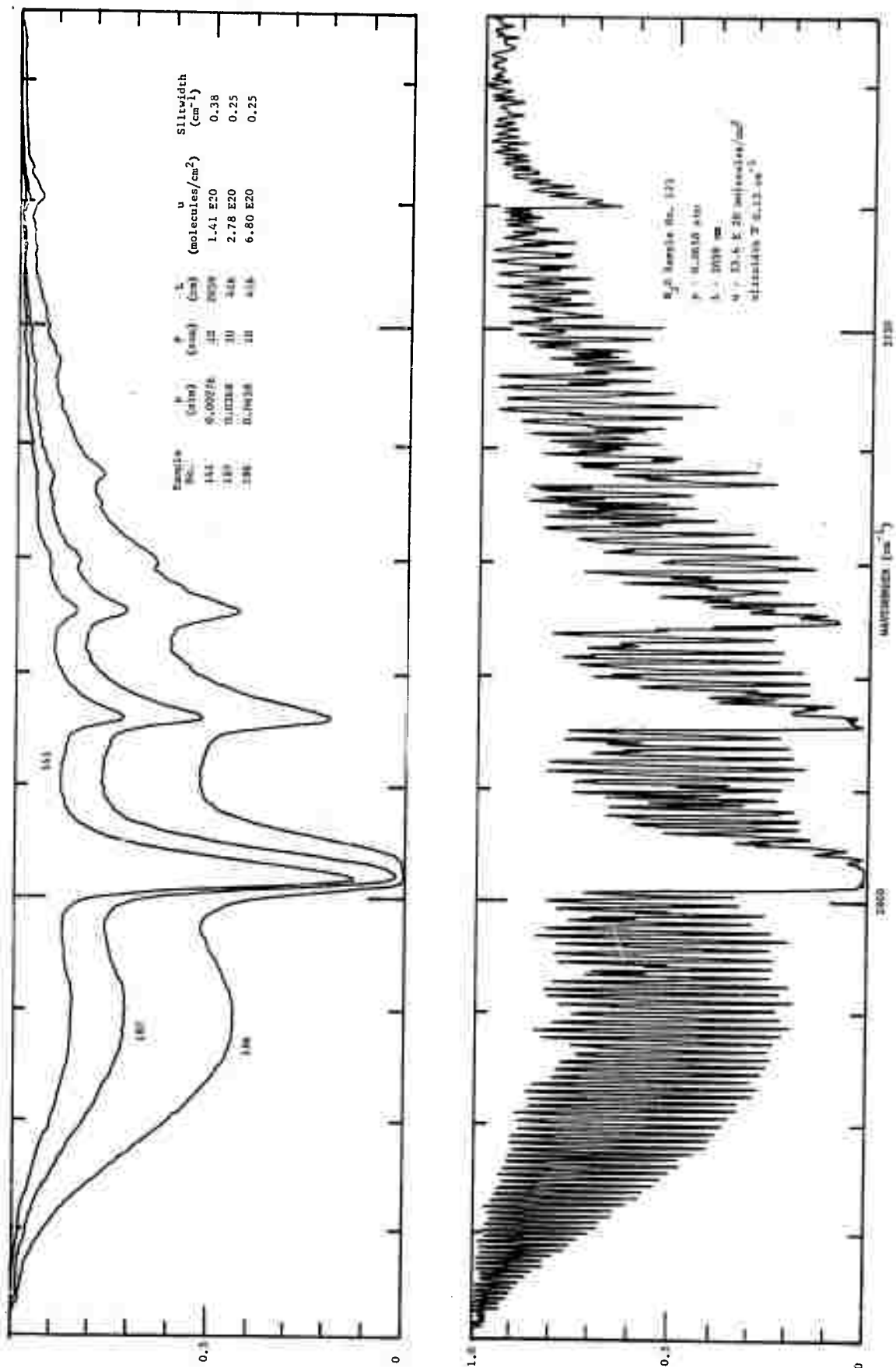


FIG. 3-21. Spectral plots of transmittance from 2725 to 2840 cm⁻¹ for N₂O samples at 296 K. The upper curves are for samples pressurized to 10 atm with N₂. The lower curve is for a pure N₂O sample. The sample parameters as well as the spectral slitwidth used are listed in the panels.

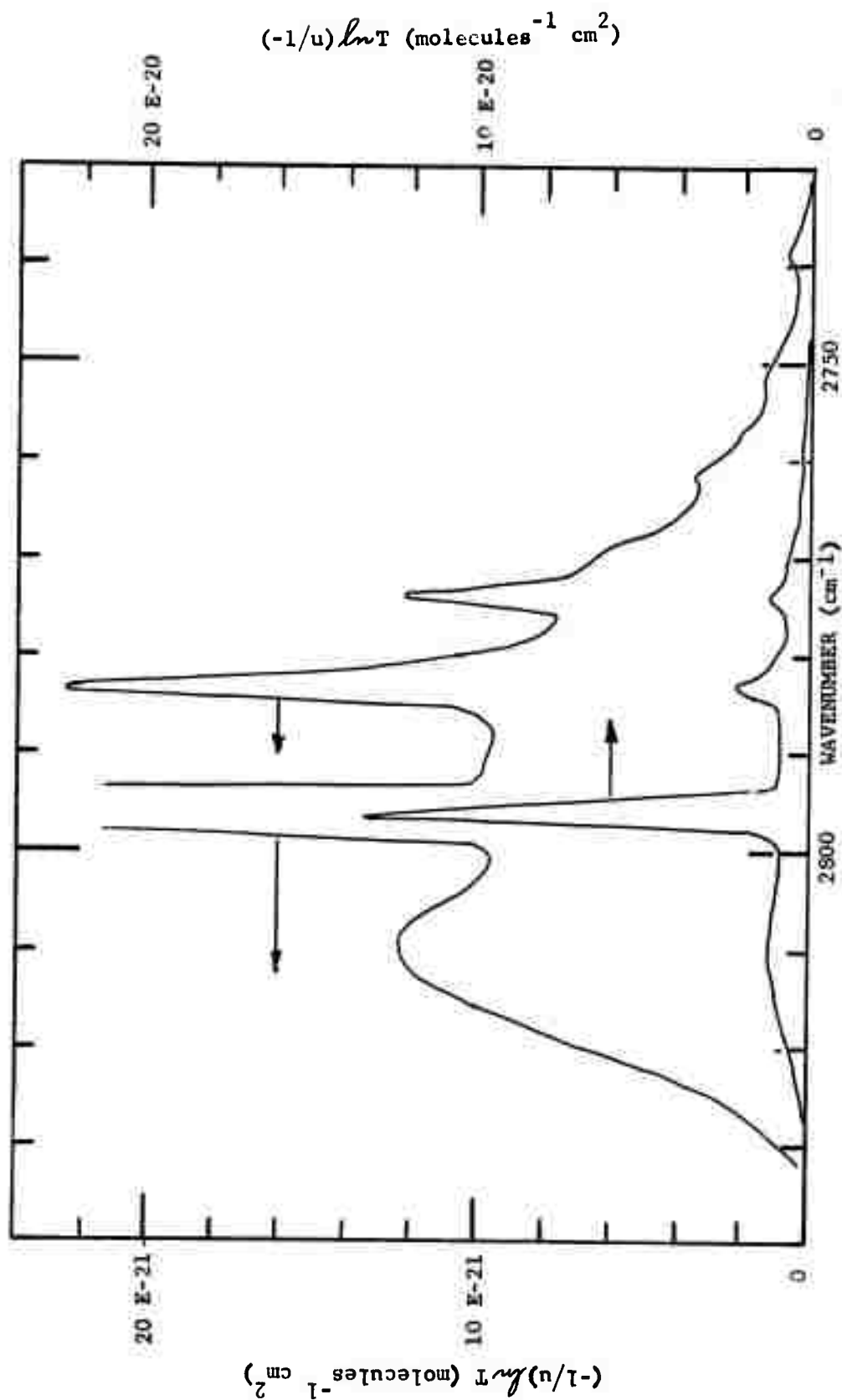


FIG. 3-22. Spectral curve of $(-1/u) \ln T$ for samples of $N_2O + N_2$ at 10 atm. The arrows indicate which ordinate scale to use.

2840-2930 cm⁻¹

The main absorption in this spectral region is due to the $10^0_1-01^1_0$ cross-over band centered at 2892.054 cm^{-1} . Other bands are $05^1_0-00^0_0$, $11^1_1-02^0_0$, $11^1_1-02^0_0$, $06^2_0-01^1_0$ and $06^0_0-01^1_0$ centered at 2897.78 , 2893.845 , 2884.229 , 2885.723 and 2877.803 cm^{-1} , respectively. The Q-branches due to these transitions are evident in Fig. 3-23. We measured the intensity of the R-branch, the combination of the P- and Q-branches, and the total intensity of the $10^0_1-01^1_0$ band. The values in $\text{molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$ are as follows with $\pm 5\%$ uncertainty:

$$S_R = 0.0071 \times 10^{-20}$$

$$S_{Q,P} = 0.0238 \times 10^{-20}$$

$$S_V = 0.0309 \times 10^{-20}$$

The relative intensities agree well with those calculated by L. D. Gray-Young.⁷ According to Young's calculations, the Q-branch is expected to have an intensity of $0.016 \times 10^{-20} \text{ molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$, which is below the limit for the line parameter listing. We also made a rough measurement on the Q-branch of the 05^1_0 band and found that its intensity is less than $0.0013 \times 10^{-20} \text{ molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$.

2930-3090 cm⁻¹

The main band ($13^1_0-00^0_0$) in this region is centered at 3046.213 cm^{-1} . The Q-branches of the associated difference bands, $14^2_0-01^1_0$ and $14^0_0-01^1_0$ centered at 3042.883 and 3032.174 cm^{-1} , respectively, are evident in Fig. 3-24. These bands are much too weak to be included in the line parameter tables; however, we measured them to compare the relative intensities with theoretical predictions. The intensities with $\pm 10\%$ uncertainty in $\text{molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$ are:

$$S_Q (13^1_0-00^0_0) = 0.0060 \times 10^{-20}$$

$$S_Q (14^2_0-01^1_0) = 0.00077 \times 10^{-20}$$

$$S_Q (14^0_0-01^1_0) = 0.00050 \times 10^{-20}$$

The R-branch of the $13^1_0-00^0_0$ band is obviously much more intense than the P-branch. Therefore, the relative intensities of the lines cannot be calculated from simple theoretical equations that do not account for vibration-rotation interactions.

3090-3210 cm⁻¹

The prominent absorption features seen in Fig. 3-25 in this region are due to the $21^1_0-00^0_0$ and $00^0_2-10^0_0$ bands centered at 3165.857 and

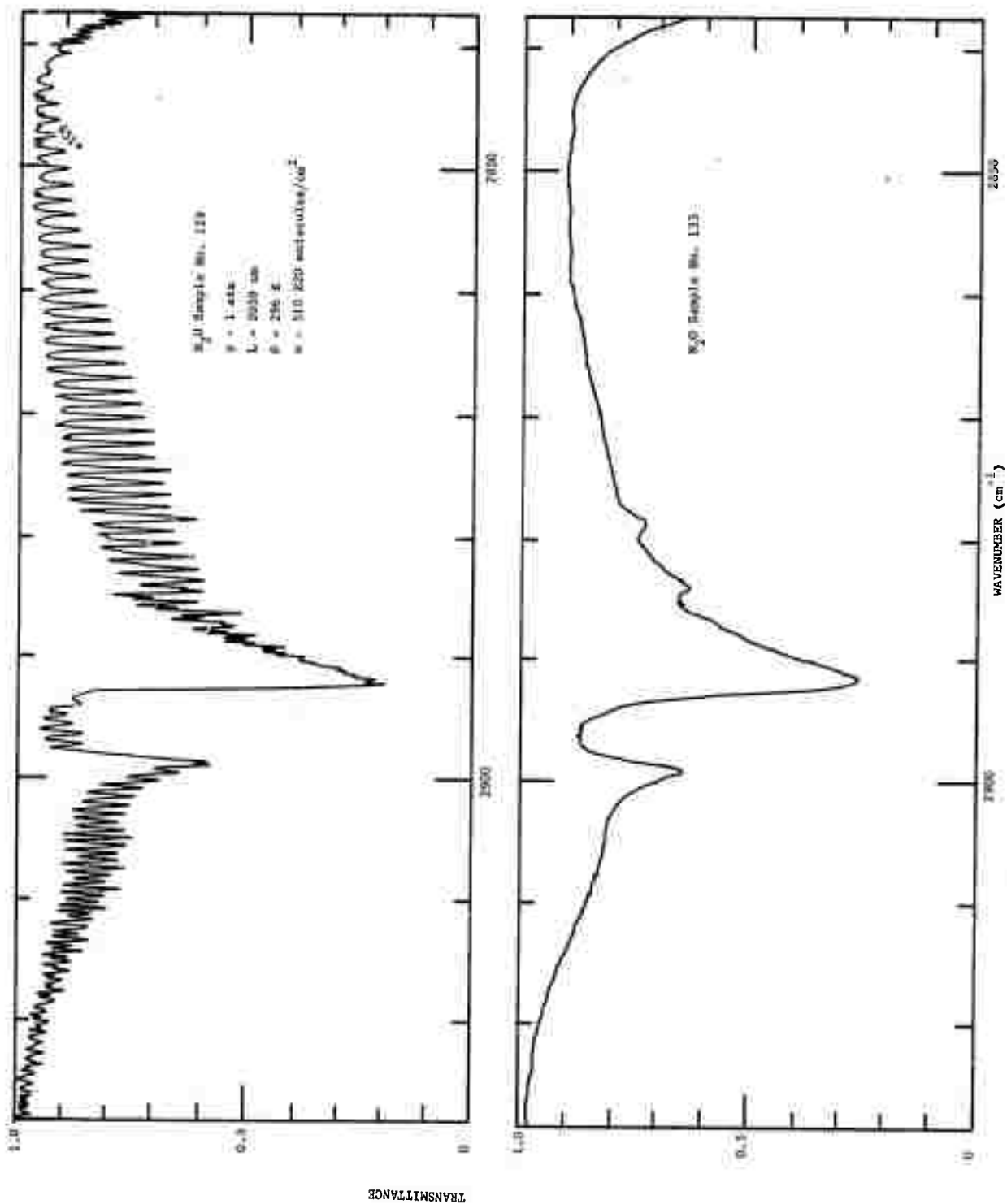


FIG. 3-23. Spectral curves of transmittance from 2840 to 2930 cm^{-1} . The sample parameters are given in the upper panel. The lower panel shows the transmittance curve for the same sample as the upper panel, except that the total pressure was increased to 10 atm with N_2 . Spectral slitwidth $\approx 0.15 \text{ cm}^{-1}$.

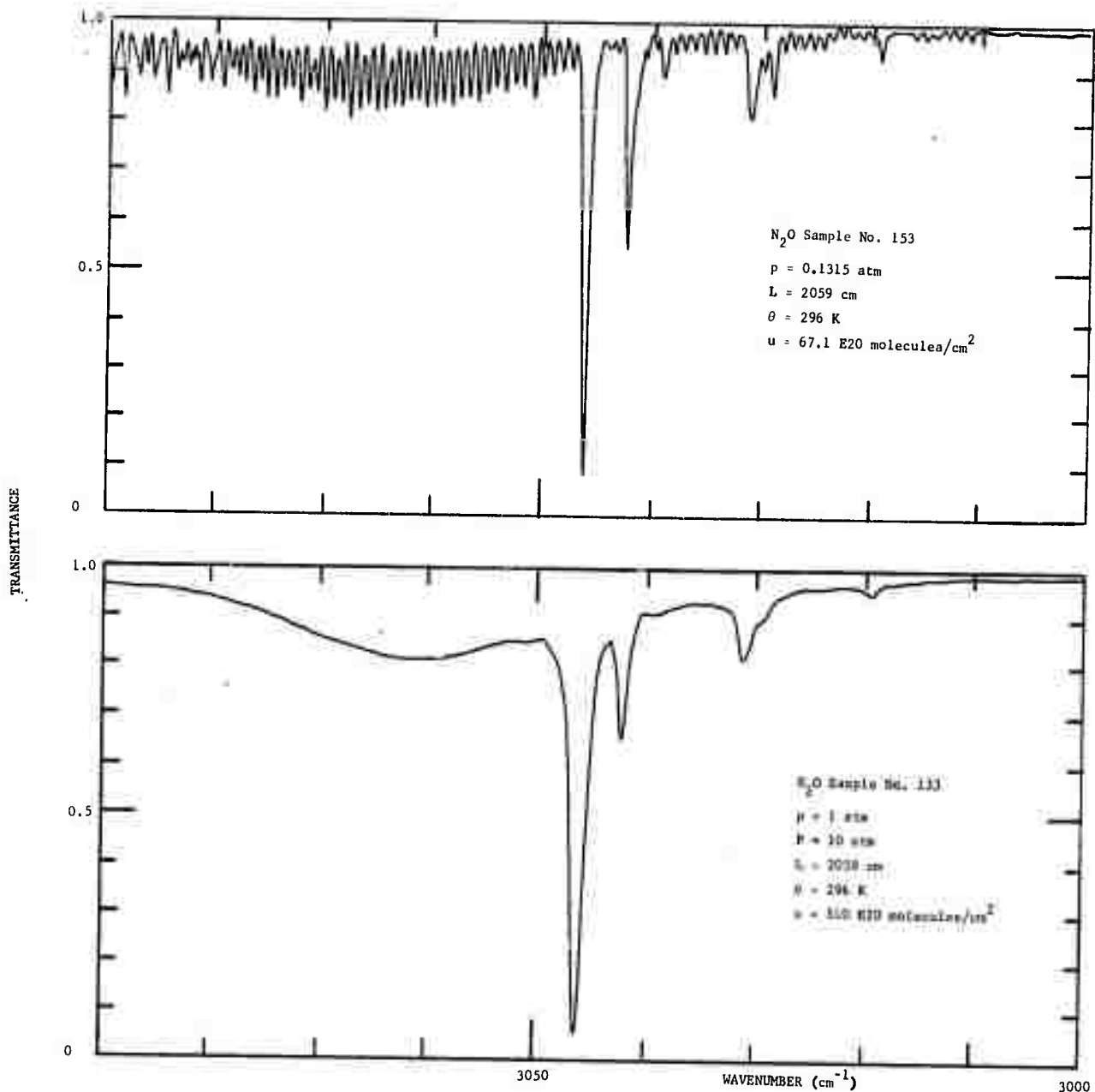


FIG.3-24. Spectral curves of transmittance from 3000 to 3090 cm^{-1} for N_2O samples at 296 K. The sample parameters are listed in the panel. Spectral slitwidth ≈ 0.17 cm^{-1} .

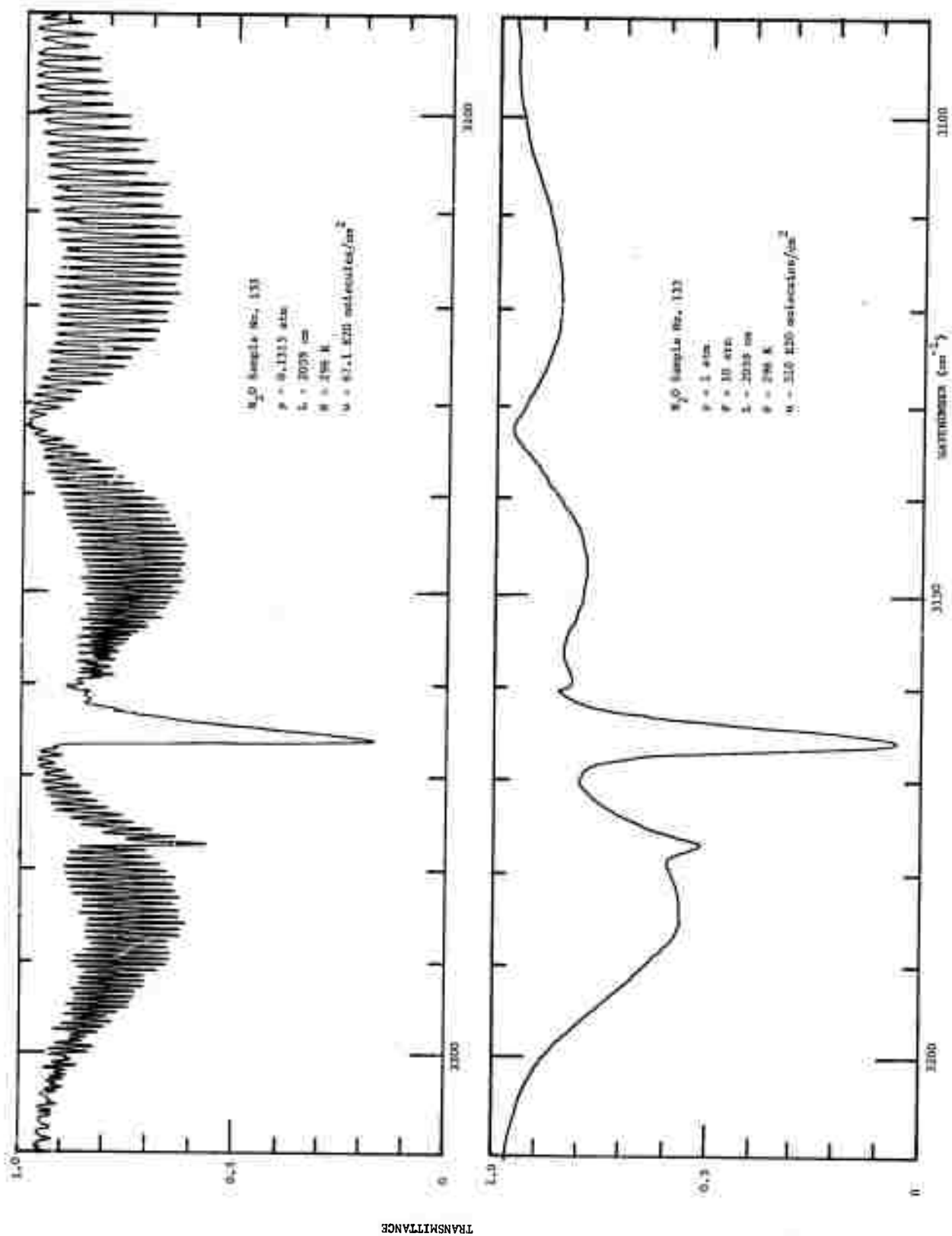


FIG. 3-25. Spectral curves of transmittance from 3090 to 3210 cm^{-1} for N_2O samples at 296 K. The sample parameters are listed in the panels. Spectral slitwidth ≈ 0.18 cm^{-1} .

3132.472 cm^{-1} , respectively. Also evident are the Q-branches of the $22^2_0\leftarrow 01^1_0$ and $22^0_0\leftarrow 01^1_0$ bands centered at 3177.293 and 3159.485 cm^{-1} , respectively.

The P-branch of the $21^1_0\leftarrow 00^0_0$ band blends into the R-branch of the $00^0_2\leftarrow 10^0_0$ crossover band. The contour of the $21^1_0\leftarrow 00^0_0$ band is not normal for a $\Pi\leftarrow\Sigma$ band. The R-branch is enhanced at the expense of the P-branch, suggesting that a correction is required to account for vibration-rotation interactions. The intensity of the P-branch was determined from the transmittance curves by estimating the contribution by the R-branch of the $00^0_2\leftarrow 10^0_0$ band and accounting for it. The intensities of the three branches in molecules $^{-1} \text{cm}^2 \text{cm}^{-1}$ are:

$$S_P(21^1_0\leftarrow 00^0_0) = 0.004 \text{ E-20} \pm 50\%$$

$$S_R(21^1_0\leftarrow 00^0_0) = 0.027 \text{ E-20} \pm 10\%$$

$$S_Q(21^1_0\leftarrow 00^0_0) = 0.012 \text{ E-20} \pm 10\%.$$

3210-3405 cm^{-1}

High resolution spectra of this region, which contains the 02^0_1 band system, are shown in Fig. 3-26. Spectra of 3 samples at the same equivalent pressure appear in Fig. 3-28. By the use of the line positions given by Tidwell, Plyler and Benedict,¹⁵ it was possible to identify lines due to the transitions $02^0_1\leftarrow 00^0_0$, $03^1_1\leftarrow 01^1_0$, $03^1_1\leftarrow 01^1_0$, $04^0_0\leftarrow 02^0_0$ and $04^2_0\leftarrow 02^2_0$.

Extra care was taken to remove most of the residual H_2O from the samples. No attempt was made to account for the remaining H_2O absorption in the main part of the N_2O bands. Corrections were made in the region between the bands where H_2O absorption was obvious.

3405-3520 cm^{-1}

The 10^0_1 band system, which occurs in this spectral region, is the strongest between 3300 and 4000 cm^{-1} . The lines due to several sub-bands can be observed in Fig. 3-29. Included are the $11^1_1\leftarrow 01^1_0$, $11^1_1\leftarrow 01^1_0$, $04^0_1\leftarrow 02^0_0$, $14^2_1\leftarrow 02^2_0$, $14^2_1\leftarrow 02^2_0$ and $20^0_1\leftarrow 10^0_0$ sub-bands in addition to the $10^0_1\leftarrow 00^0_0$ bands of the isotopes $^{14}\text{N}^{15}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{14}\text{N}^{16}\text{O}$. Figure 3-30 shows a spectrum of a high-pressure sample and a plot of $(-1/u) \ln T$ for the same sample with the structure smoothed out. The structure in the P-branch was not completely smoothed out by the pressure broadening. We used pre-mixed samples of 2.19% and 4% N_2O in N_2 at a total pressure of 7.8 atm to measure the intensity of the band system. The sample cell length was 3.96 cm. Values of $(-1/u) \ln T$ for the two samples compared very well. Spectral curves representing 3 samples of different absorber thickness at the same equivalent pressure are shown in Fig. 3-31.

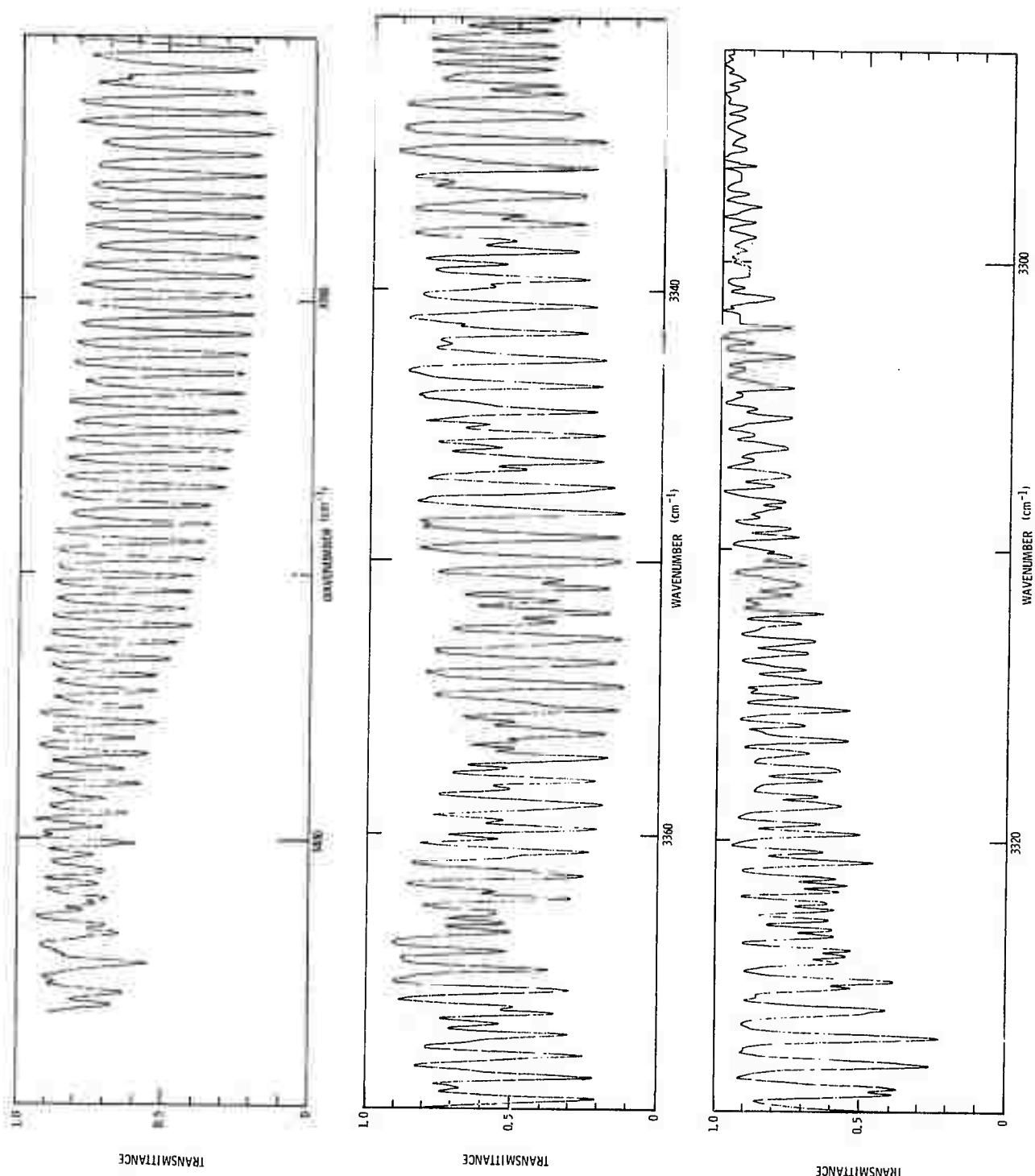


FIG. 3-26. Spectral curve of transmittance from 3292 to 3410 cm^{-1} . Sample 302. $p = 0.132 \text{ atm}$, $L = 416 \text{ cm}$, $u = 13.6 \text{ E 20 molecules/cm}^2$, spectral slitwidth = 0.17 cm^{-1} .

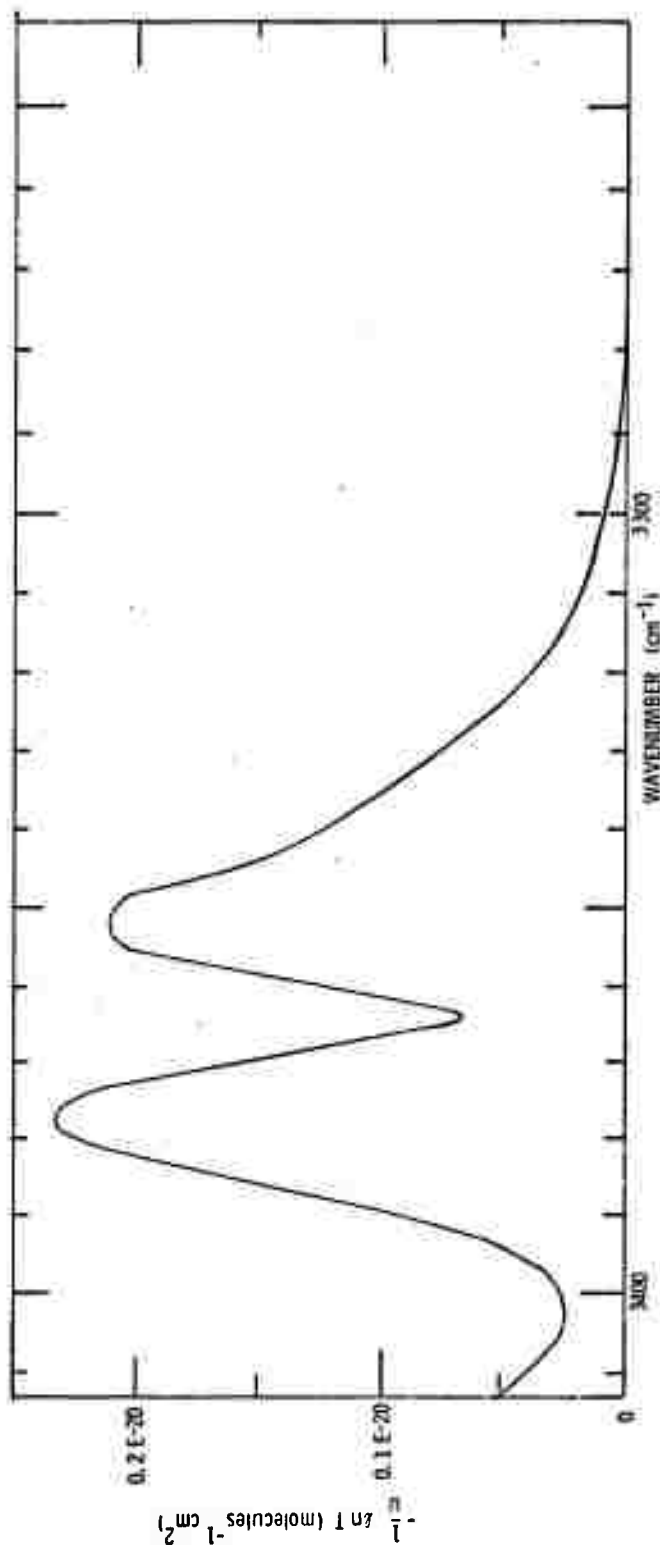
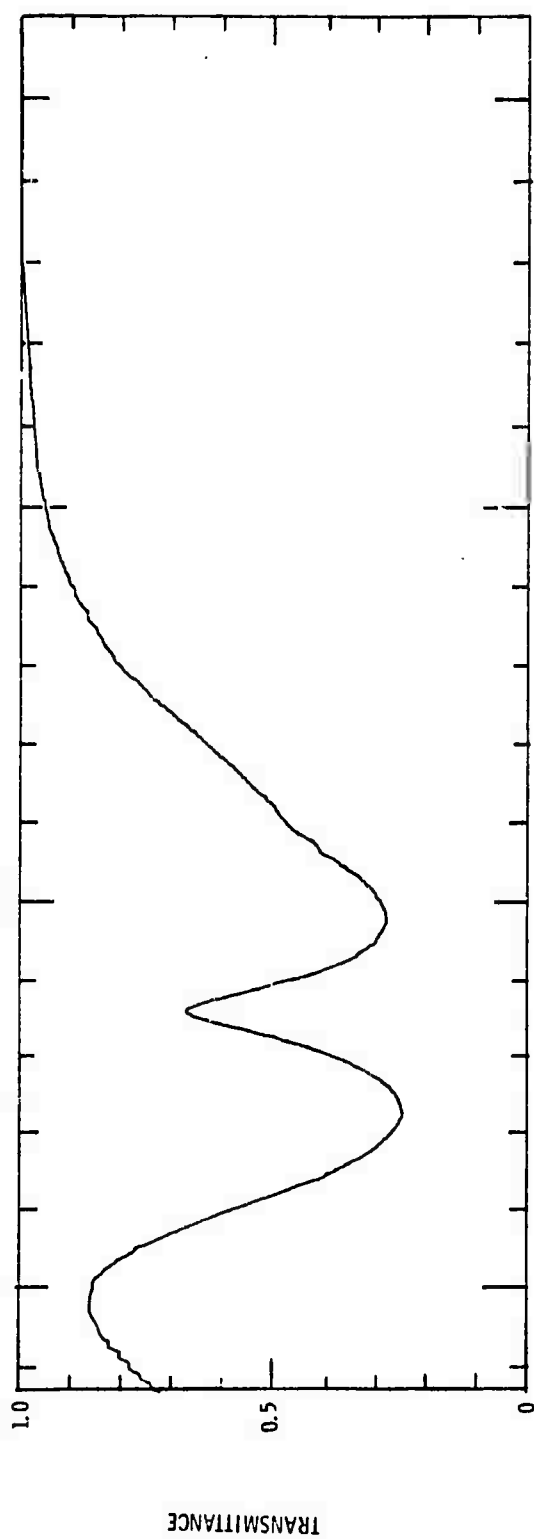


FIG. 3-27. Spectral curves of transmittance and $(-1/u) \ln T$ from 3240 to 3410 cm^{-1} . Sample 277, $p = 6 \text{ atm}$, $P = 6 \text{ atm}$, $L = 3.96 \text{ cm}$, $u = 6.07 \text{ E20 molecules/cm}^2$, spectral slitwidth = 0.75 cm^{-1} .

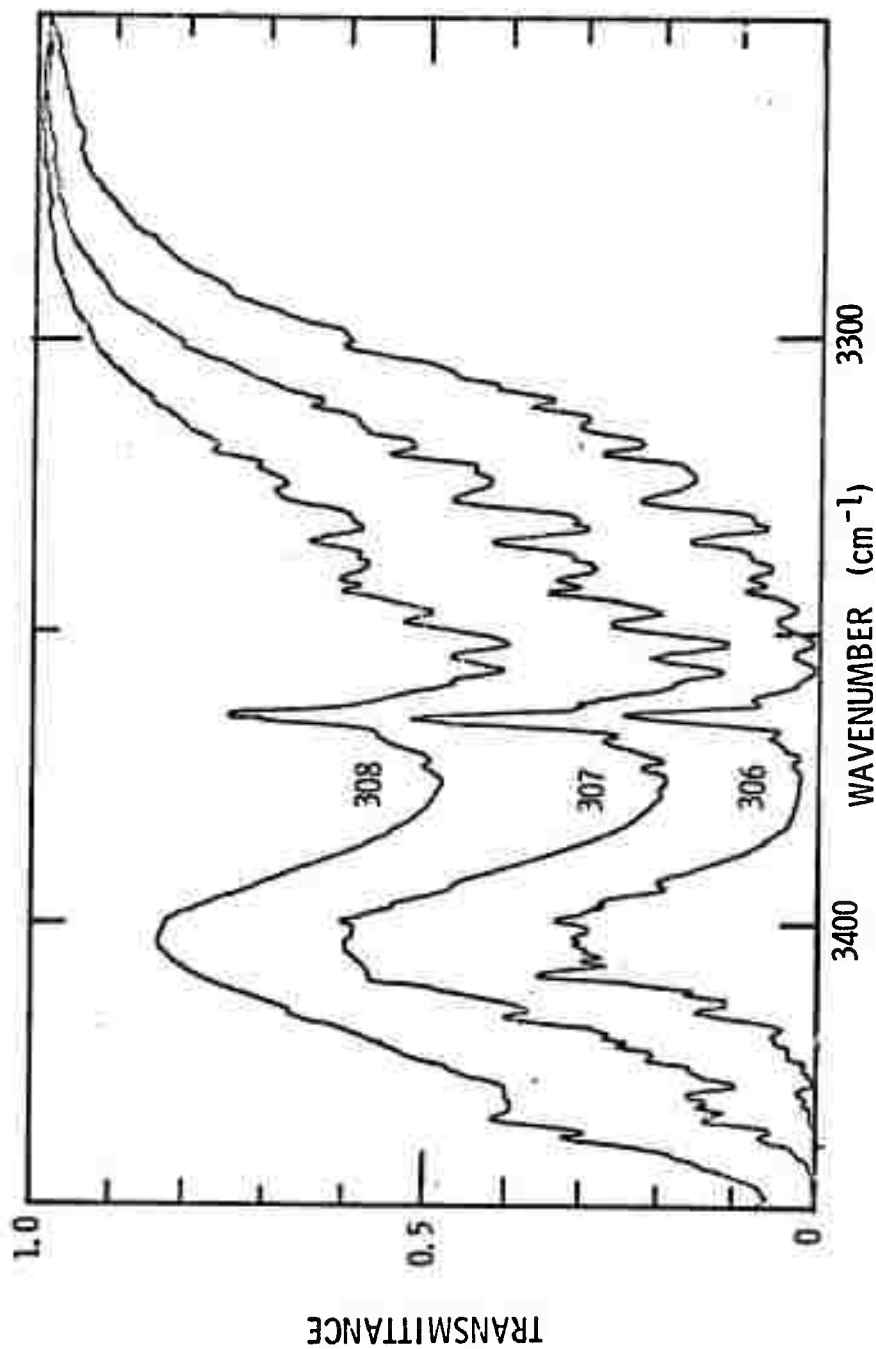


FIG. 3-28. Spectral curves of transmittance from 3250 to 3450 cm^{-1} for 3 samples.

Sample No.	p atm	P atm	P _e atm	u molecules/cm ²
306	0.24	0.24	0.30	99.1 E20
307	0.08	0.28	0.30	32.8 E20
308	0.024	0.295	0.30	9.90 E20

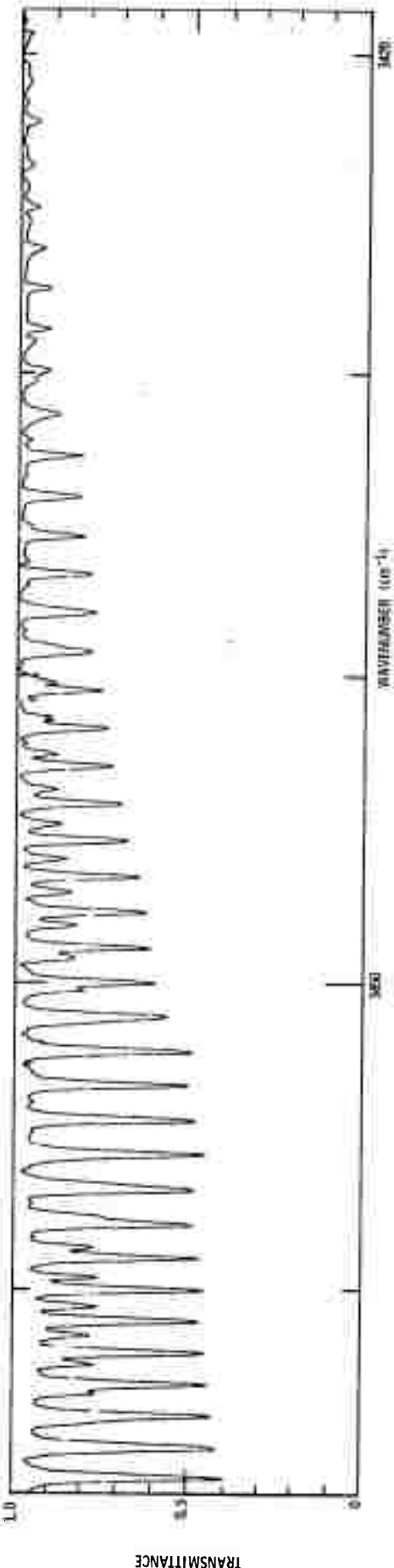
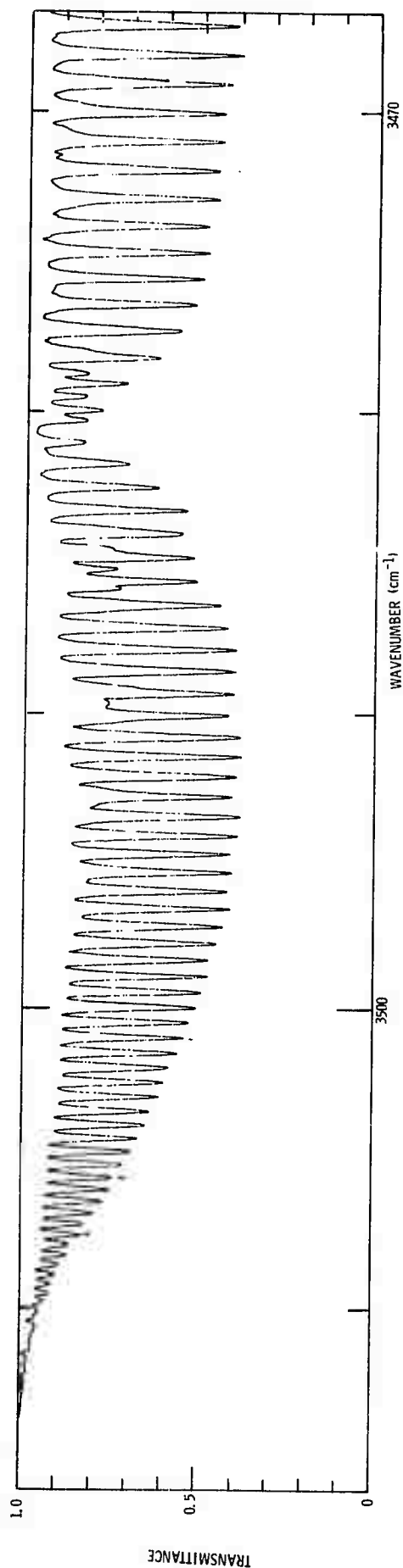


FIG. 3-29. Spectral curve of transmittance from 3420 to 3520 cm^{-1} . Sample 289, $p = 0.312$ at m, $L = 3.96$ cm, $u = 0.129$ E 20 molecules/ cm^2 , spectral slitwidth = 0.18 cm^{-1} .

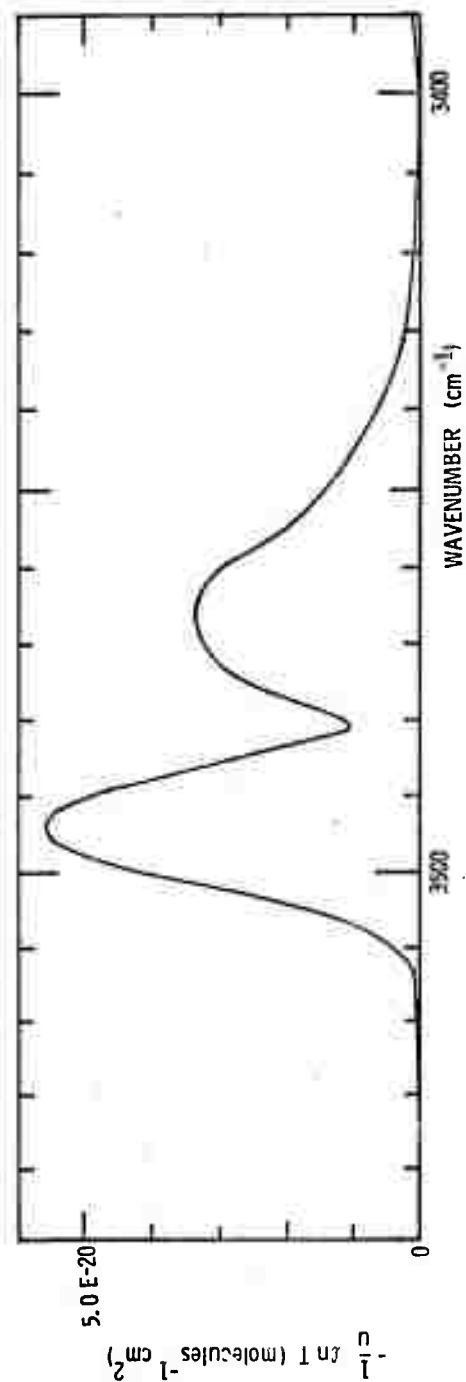
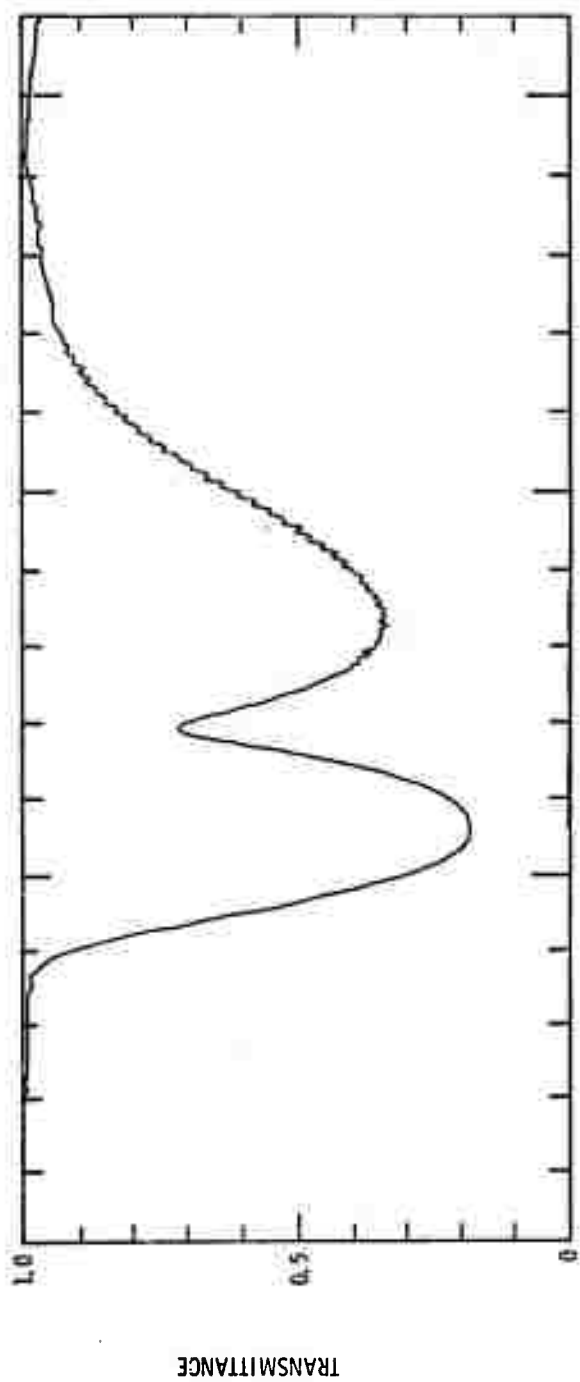


FIG. 3-30. Spectral curves of transmittance and $(-1/u) \ln T$ from 3390 to 3550 cm⁻¹. Sample 301, $p = 0.312$ atm, $P = 7.8$ atm, $L = 3.96$ cm⁻¹, $u = 0.307$ E20 molecules/cm², spectral slitwidth = 0.5 cm⁻¹.

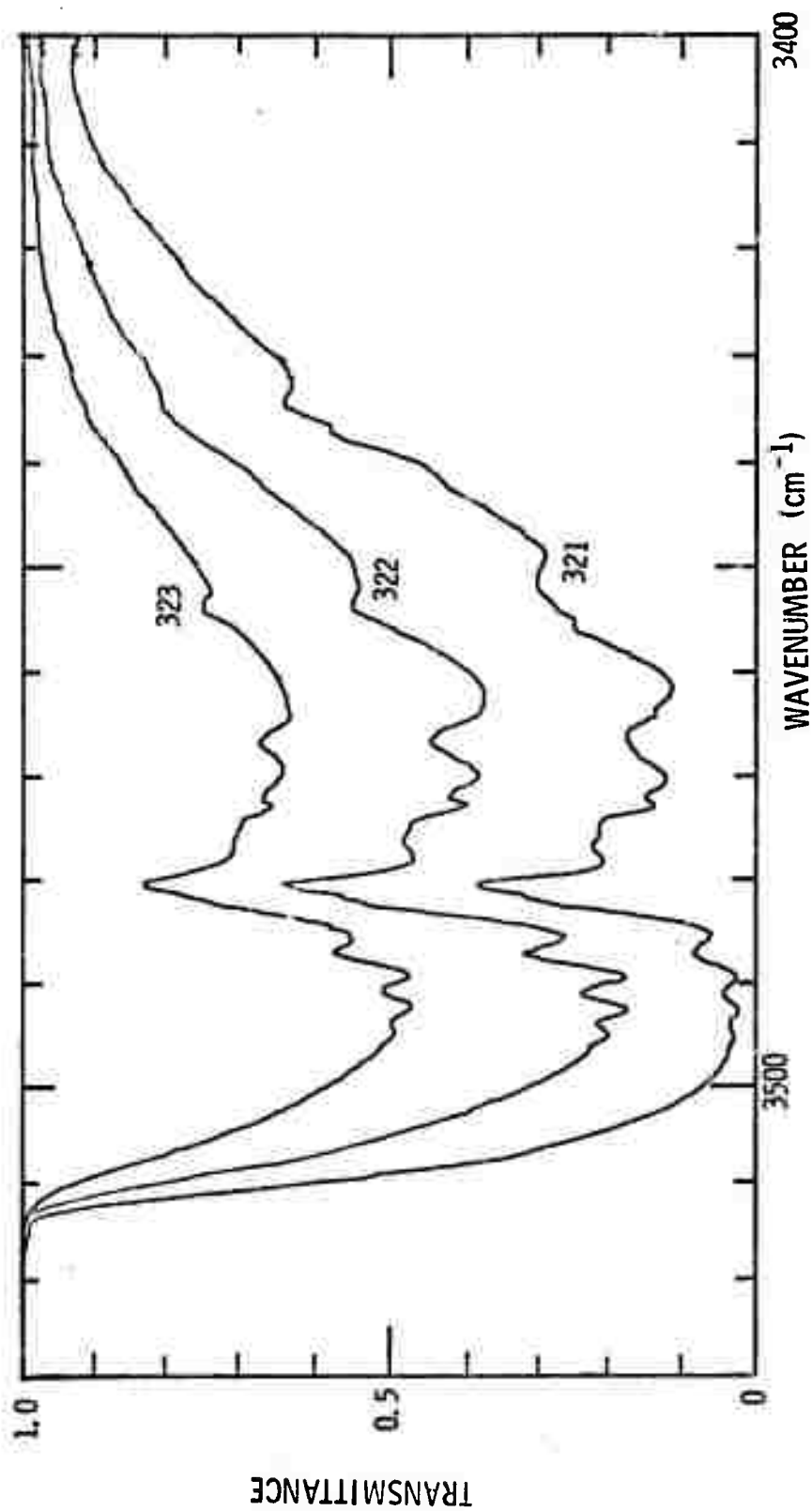


FIG. 3-31. Spectral curves of transmittance from 3400 to 3530 cm^{-1} for 3 samples.

Sample No.	P atm	P atm	P _e atm	U molecules/cm ²
321	0.0320	0.282	0.29	3.30 E20
322	0.0107	0.287	0.29	1.10 E20
323	0.00316	0.290	0.29	0.326 E20

The R45 and P47 lines of the 06^0_0 band were observed by Tidwell et al¹⁵ and by Toth⁶ and found to have anomalously high intensities. Toth also observed some lines due to the forbidden band 06^2_0 . The rotational levels $J' = 46$ for the 06^0_0 and 10^0_1 vibrational levels are close enough together that Fermi-interaction becomes important with the result that the intensities of the R45 and P47 lines of the 06^0_0 band are enhanced and the positions are shifted. The rotational lines R27 and P29 of the 06^2_0 are also enhanced and shifted due to the Fermi interaction of the $J' = 28$ rotational level of the 06^2_0 and 10^0_1 vibrational levels. The intensities of the remainder of the lines of the 06^0_0 and 06^2_0 bands are much less than our limit ($0.004 \text{ E-20 molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$) for inclusion in the line parameter listing.

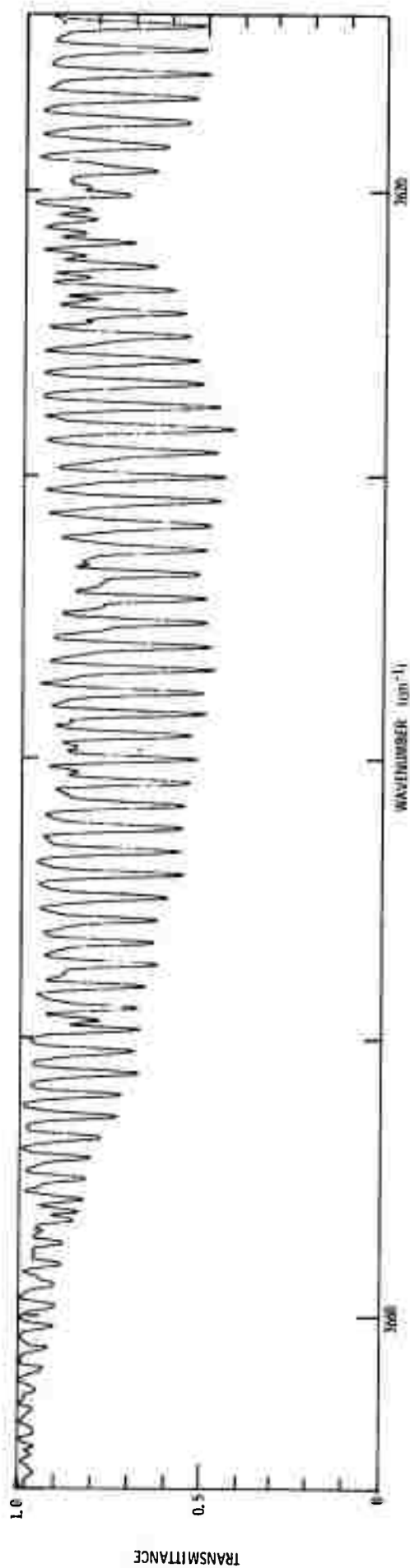
The values of the perturbed line positions and intensities as determined from Toth and Tidwell et al are given in the table below.

TABLE 3-2
PERTURBED INTENSITIES AND POSITIONS
OF LINES OF 10^0_1 , 06^0_0 and 06^2_0 BANDS

Line	Band	ν_o cm^{-1}	S_J $\text{molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$ Multiply by E-20
R45	10^0_1	3508.028	0.0225 ± 0.007
R45	06^0_0	3508.184	0.042 ± 0.0012
P47	10^0_1	3430.230	
P47	06^0_0	3430.400	
R27	10^0_1	3500.040	1.89 ± 0.07
R27	06^2_0	3500.110	0.021 ± 0.001
P29	10^0_1	3452.316	
P29	06^2_0	3452.386	

3520-3670 cm^{-1}

Figures 3-32, 3-33 and 3-34 show spectral plots of transmittance and of $(-1/u) \ln T$ for this spectral region which contains the 14^0_0 band system. The original transmittance curve of the sample shown in Fig. 3-33 had some obvious low-pressure H_2O lines that were removed before replotting it. However, some additional absorption by H_2O in the sample probably exists near 3683 cm^{-1} . We did not correct the curve for this absorption. A band (20^0_1 - 02^0_0) near 3562 was identified but too weak to be included in the line parameter tables and not shown in any of the figures.



3-41

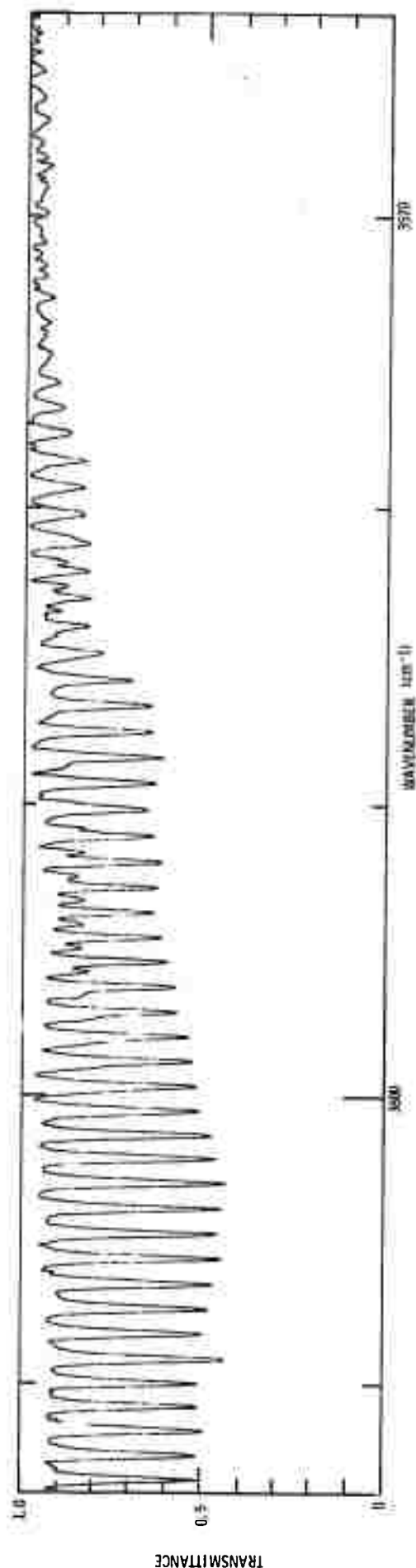
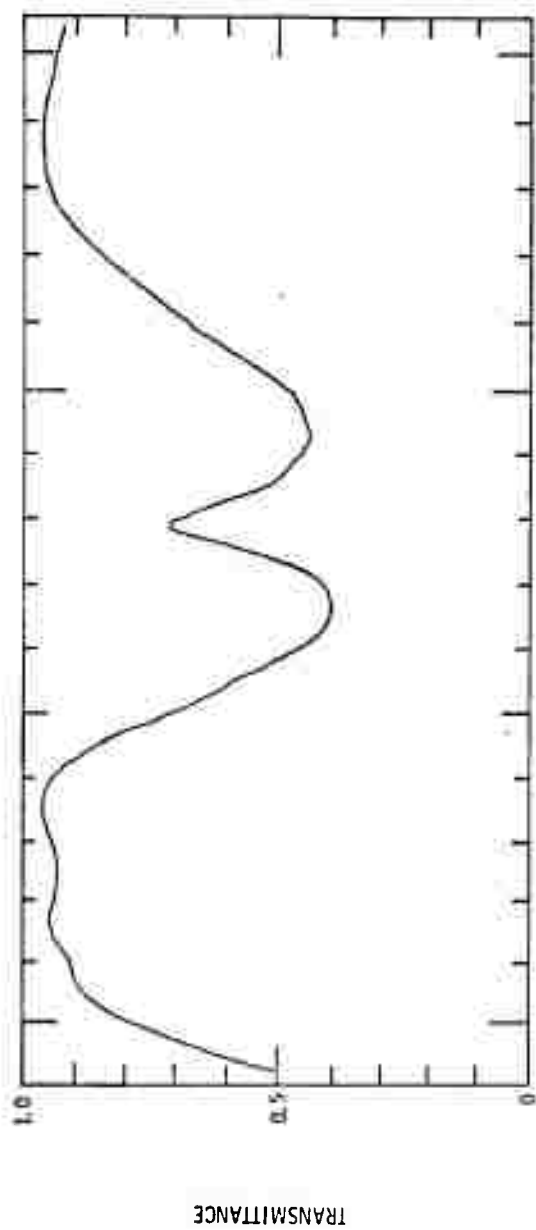


FIG. 3-32. Spectral curve of transmittance from 3560 to 3665 cm^{-1} . Sample 316, $p = 0.146 \text{ atm}$, $L = 1648 \text{ cm}$, $u = 59.7 \text{ E } 20 \text{ molecules/cm}^2$, spectral slitwidth = 0.19 cm^{-1} .



3-42

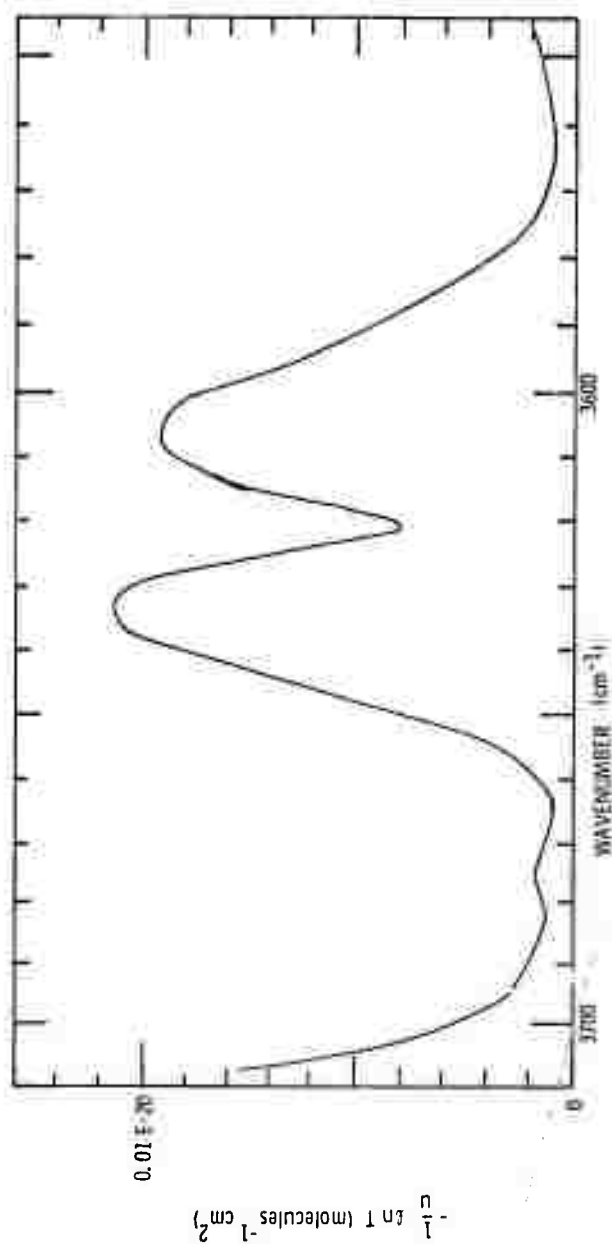


FIG. 3-33. Spectral curves of transmittance and $(-1/u) \ln T$ from 3545 to 3710 cm^{-1} . Sample 273, $p = 0.414$ atm, $P = 9.97$ atm, $L = 826$ cm, $u = 85$ E20 molecules/ cm^2 , spectral slitwidth = 0.5 cm^{-1} .

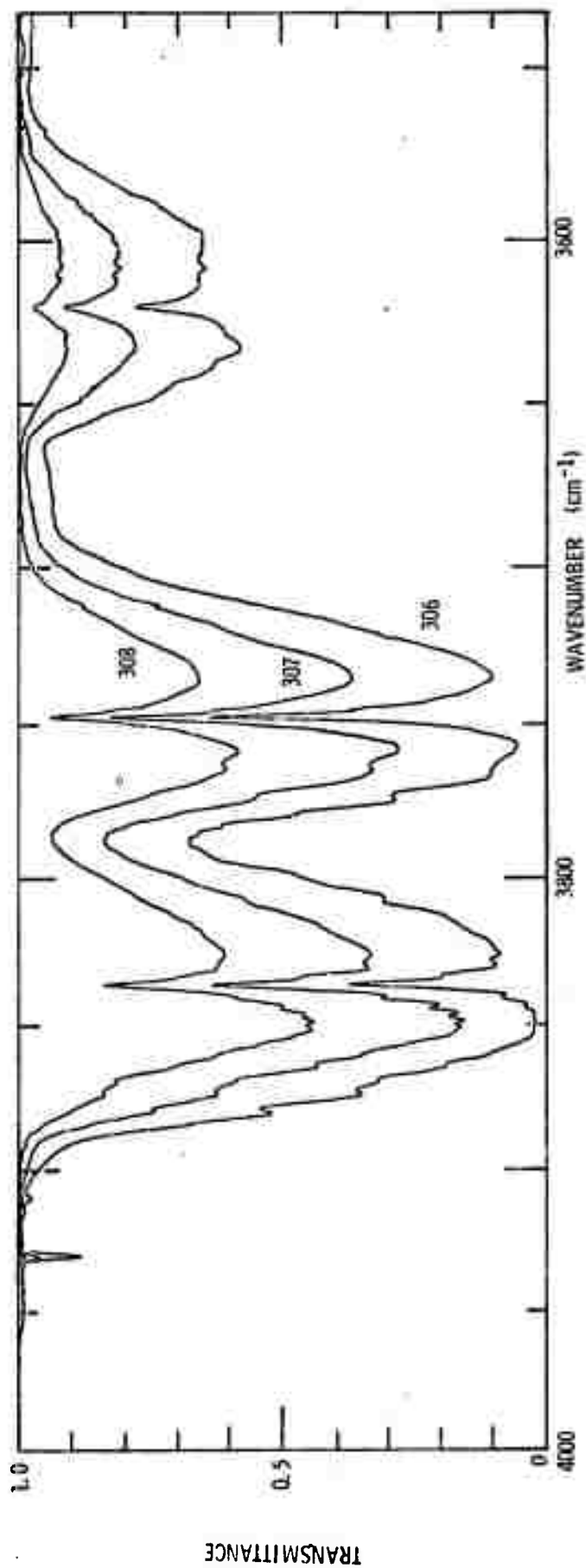


FIG. 3-34. Spectral curves of transmittance from 3540 to 4000 cm^{-1} for 3 samples.

Sample No.	p atm	P atm	P _e atm	u molecules/cm ²
306	0.24	0.24	0.30	99.1 E20
307	0.08	0.28	0.30	32.8 E20
308	0.024	0.295	0.30	9.90 E20

3670-3790 cm⁻¹

Figure 3-35 shows a spectral scan of this region obtained with about 0.2 cm⁻¹ spectral slitwidth. Some of the lines due to the main band, 22⁰0, and the 23¹0-01¹0 band are evident. Figure 3-34 shows spectral scans of 3 samples for this region. In the original spectra there were several lines that were not completely smoothed out in the P-branch of this band, even at 1.38 cm⁻¹ spectral slitwidth. The residual structure was smoothed by hand. Some large variations in the transmittance in the R-branch may be due to H₂O. We did not remove these because of the uncertainty of their source. There is evidence that not all of the structure is due to H₂O.

3790-4000 cm⁻¹

A high resolution spectrum of the main band, 30⁰0, is shown in Fig. 3-37. The wide variation in amplitude of the curves between 3870 and 3883 cm⁻¹ results from lines of the difference bands getting in and out of phase with lines of the main band. Figure 3-36 shows a spectrum for a sample at 6 atm. Values of $(-1/u) \ln T$ based on this sample compared well with those from an 8 atm sample and a 4 atm sample. The intensity of the band system is $8.15 \pm 0.4 \times 10^{-20}$ cm⁻¹ molecules⁻¹ cm². Two other bands, 40⁰0-02⁰0 and 03¹1 near 3937 and 3931 cm⁻¹ were identified but they were too weak to include in the tables.

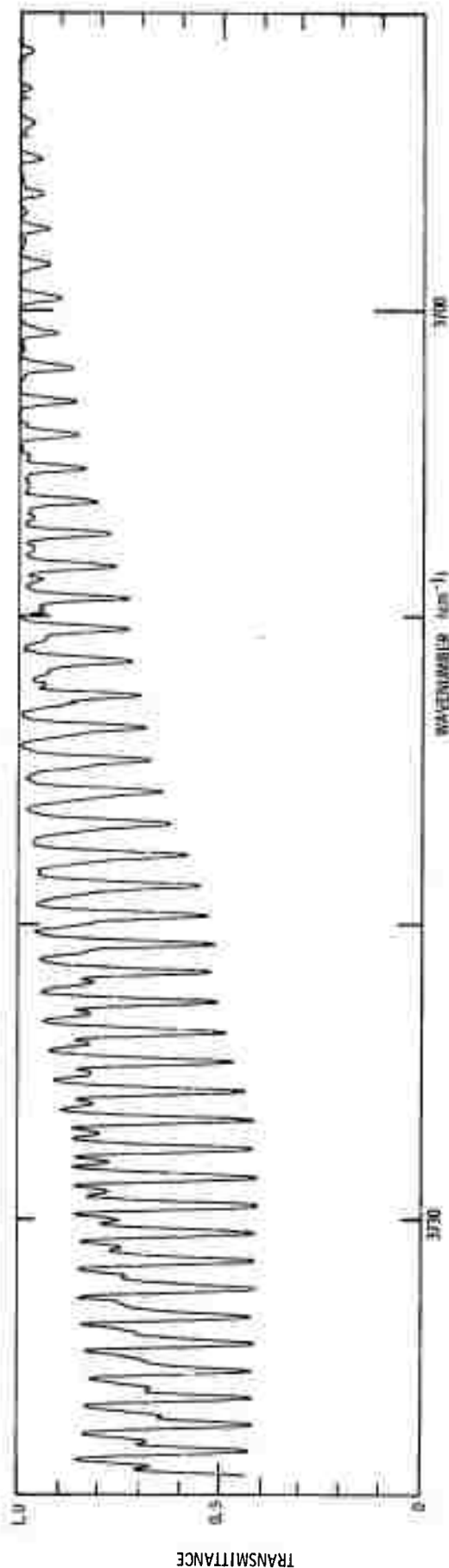
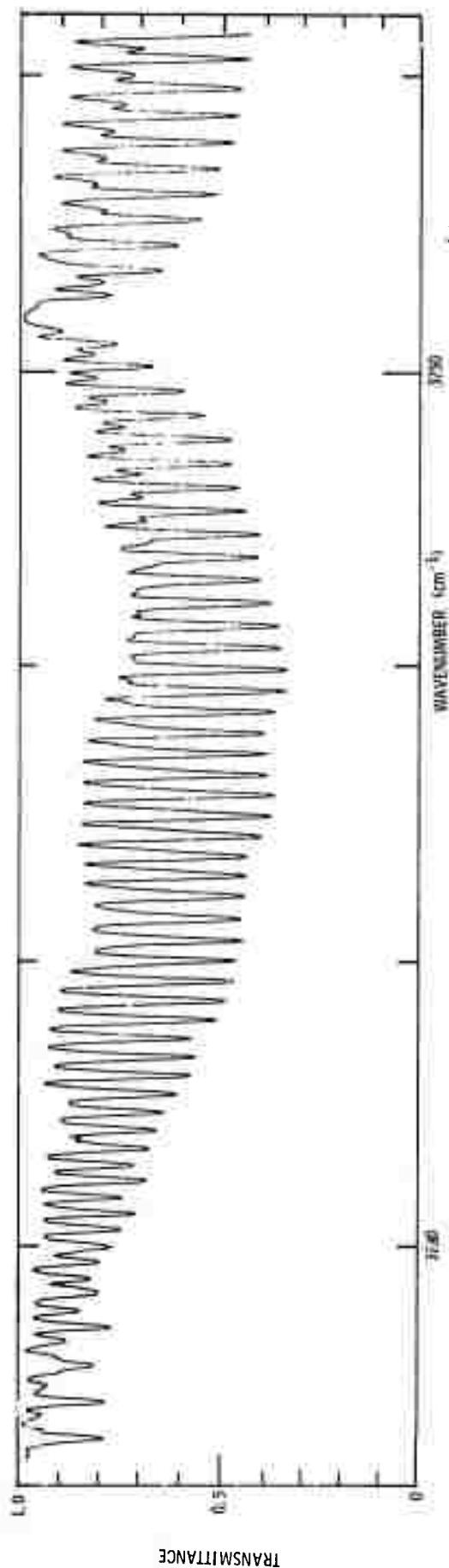


FIG. 3-35. Spectral curve of transmittance from 3600 to 3700 cm^{-1} . Sample 300, $p = 0.132$ atm, $t = 41.6$ cm, $v = 23.6$ E.20 molecules/ cm^2 . Spectral slitwidth = 0.20 cm^{-1} .

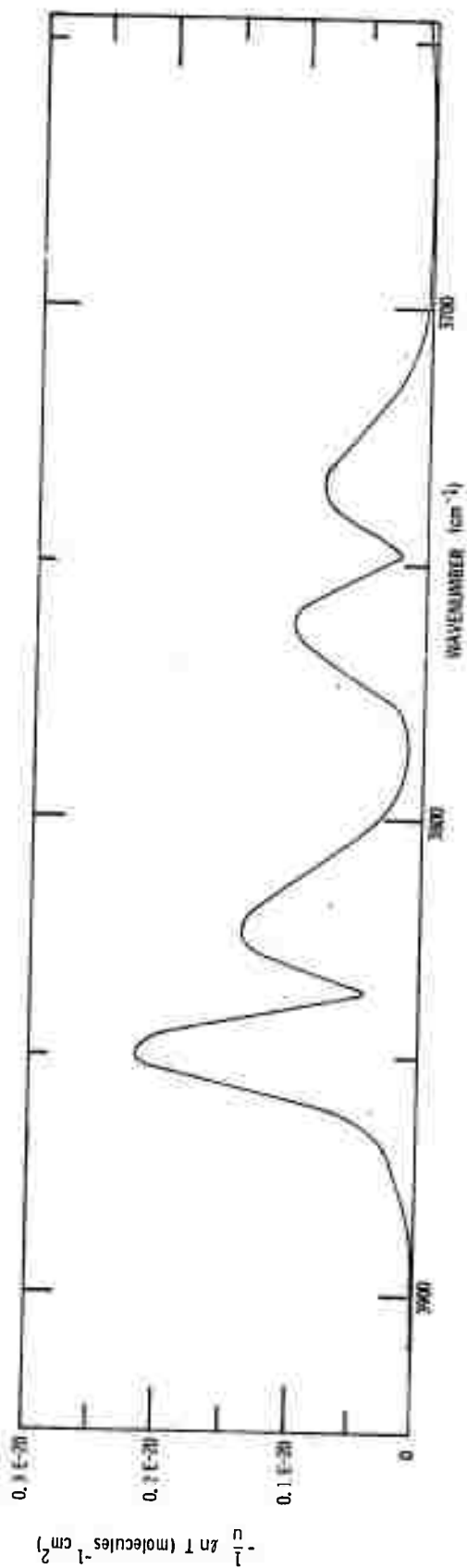
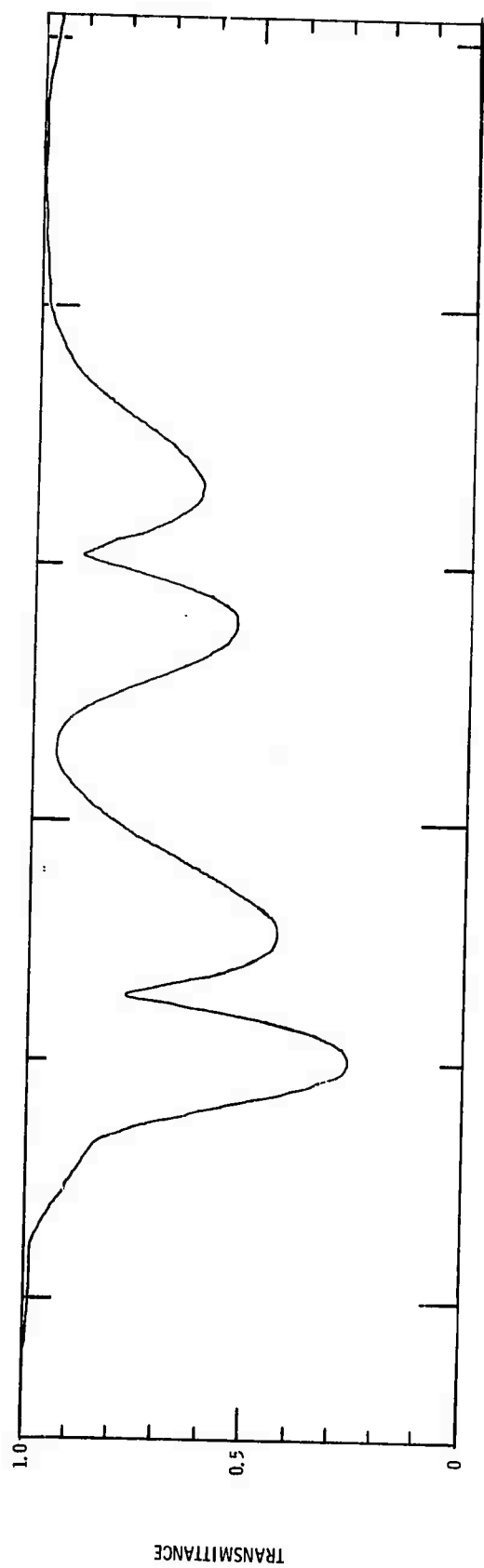


FIG. 3-36. Spectral curves of transmittance from 3650 to 3030 cm⁻¹. Sample 277, $p = 6$ atm, $L = 3.96$ cm, $u = 6.07$ E20 molecules/cm², spectral slitwidth = 0.75 cm⁻¹.

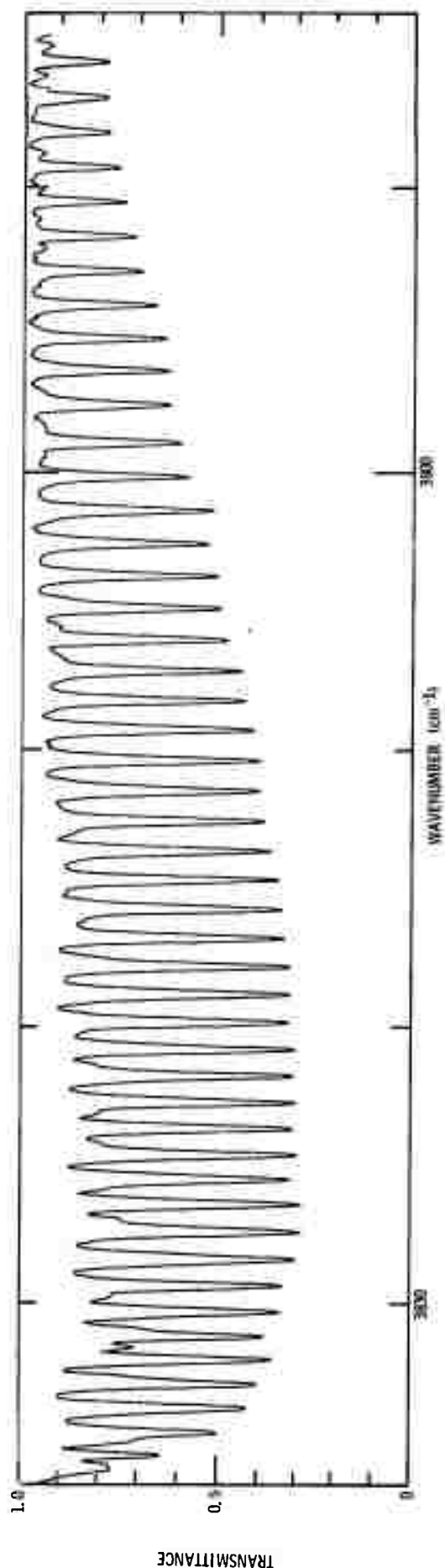
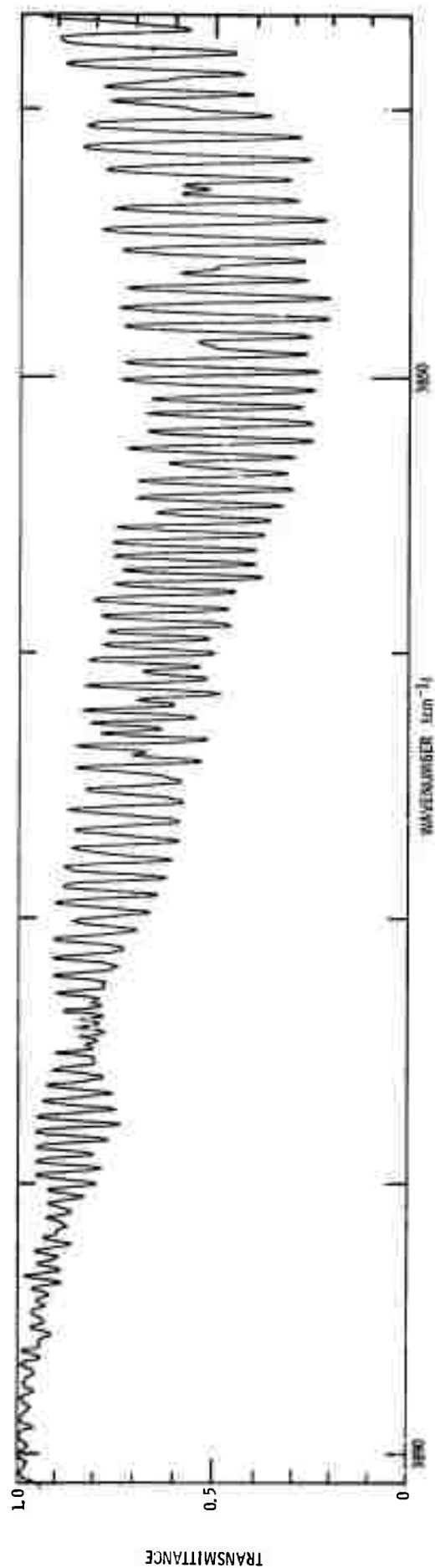


FIG. 3-37. Spectral curves of transmittance from 3785 to 3690 cm^{-1} . Sample 310, $p = 0.132$ atm, $L = 416$ cm, $u = 13.6$ E20 molecules/ cm^2 , spectral slitwidth = 0.21 cm^{-1} .

SECTION 4

DATA ON THE 530-750 cm^{-1} REGION

The spectral region from 530 to 750 cm^{-1} was investigated by using a Ge:Cu detector cooled to liquid helium temperature. A 40 line per mm grating blazed at 22.5 μm was used from 530 to 650 cm^{-1} and a 75 line per mm grating blazed at 12 μm from 650 to 750 cm^{-1} . A KBr foreprism eliminated overlapping orders. Representative spectral curves for the samples studied are shown in Figs. 4-1 through 4-4.

Figure 4-1 shows spectral curves of transmittance between 530 and 650 cm^{-1} for four N_2O samples. The $\text{N}_2\text{O} + \text{N}_2$ represented by the lower panel were mixed in a mix tank before being introduced into the sample cell to a total pressure of 6 atm. The backgrounds were determined and carefully checked for consistency with other samples before the spectra were digitized and the band intensity was determined.

The Q-branches of the $01^1_0-00^0_0$, $02^0_0-01^1_0$ and $02^2_0-01^1_0$ bands appear near their centers at 588.767, 579.367 and 588.983 cm^{-1} , respectively. The Q-branches of the $01^1_0-00^0_0$ and $02^2_0-01^1_0$ bands are nearly coincident and appear as a single feature. The Q-branch of the $02^0_0-01^1_0$ band is easily recognized. Other features result from the $03^1_0-02^0_0$ and $03^1_0-02^2_0$ bands centered at 580.924 and 571.308 cm^{-1} and from the $01^1_0-00^0_0$ bands of the 546 and 456 isotopes centered at 585.320 and 575.5 cm^{-1} , respectively.

The intensity of the system was measured to be $118 \pm 9 \text{ E-20 molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$, which compares quite well with $112 \pm 15 \text{ E-20}$ obtained by Burch and Williams.¹⁶ Sample No. 359 was used to determine the combined intensities ($55.7 \pm 6 \text{ E-20 molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$) of the Q-branches of the $01^1_0-00^0_0$ and $02^2_0-01^1_0$ bands.

The upper panel of Fig. 4-1 shows a transmittance curve for a sample at lower pressure such that much of the structure is apparent. The calibration of this spectral region was obtained using known values of CO_2 , N_2O and H_2O absorption lines as reported by Gordon et al,¹⁷ Lakshmi et al,¹⁸ and Blaine et al,¹⁹ respectively.

Figure 4-2 shows spectral curves of $(-1/u) \ln T$ for this spectral region; two different ordinate scales are used to show more detail. Transmittance curves from 650 to 750 cm^{-1} are shown in Fig. 4-3 for 3 N_2O samples. The three prominent features are due to the $10^0_0 \leftarrow 01^1_0$, $11^1_0 \leftarrow 02^0_0$ and $11^1_0 \leftarrow 02^2_0$ bands centered at 696.140, 712.134 and 702.518 cm^{-1} , respectively.

The lower panel shows representative transmittance curves from which the intensity was determined. The pressures of the samples were high enough that the line structure was smoothed out. The backgrounds were determined by comparing with other spectral curves for consistency. A small amount of absorption near 670 cm^{-1} by some residual CO_2 contaminant in the sample was accounted for. The intensity of the system was determined to be $0.354 \pm 0.02 \text{ E-20 molecules}^{-1} \text{ cm}^2 \text{ cm}^{-1}$.

Known published values^{17,20,21} of CO_2 line positions were used to calibrate this spectral region.

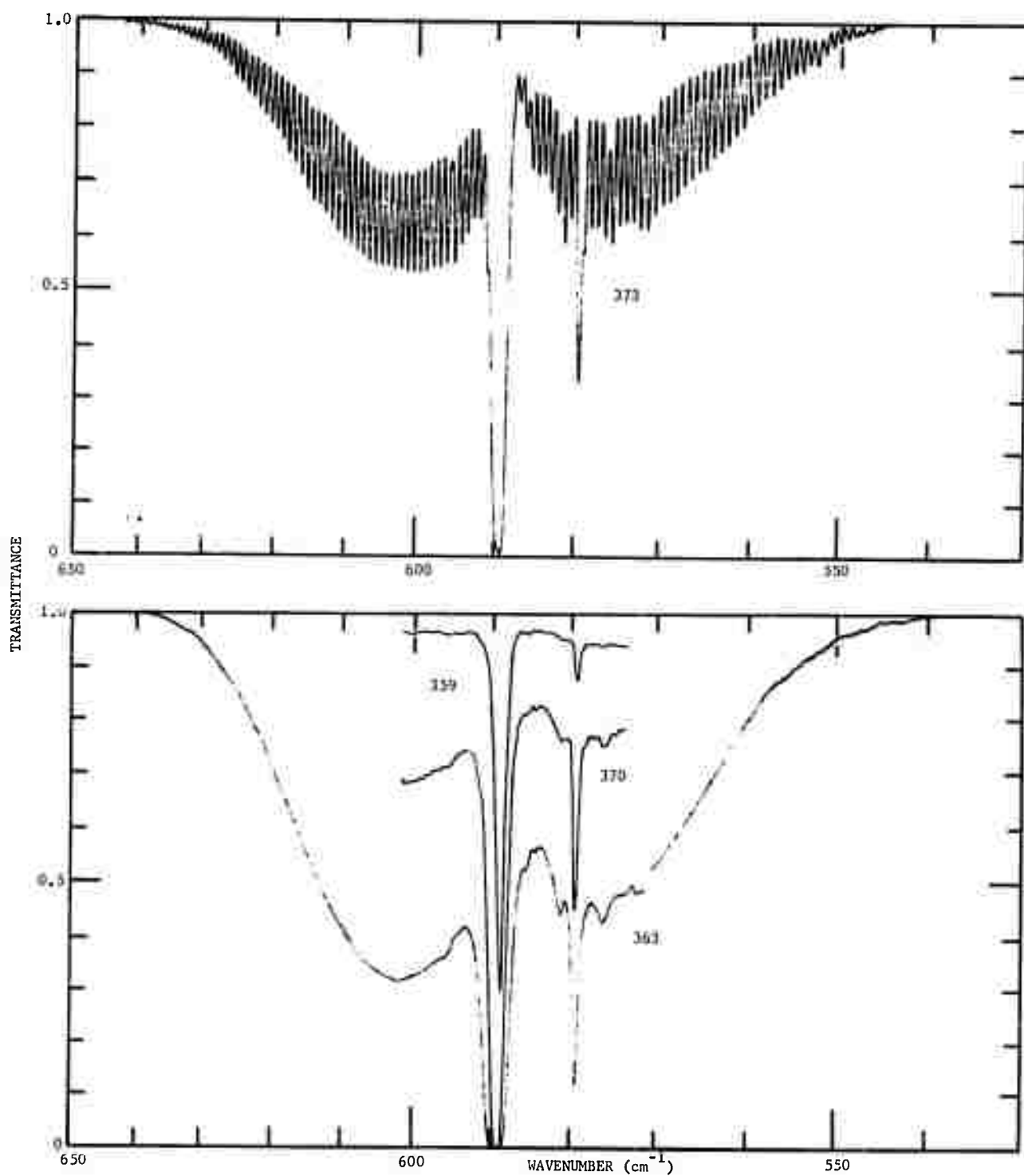


FIG. 4-1. Spectral curves of transmittance from 530 to 650 cm⁻¹ for 4 N₂O samples.

Sample No.	p atm	P atm	L cm	u molecules/cm ²	Slitwidth cm ⁻¹
363	0.72	6	3.96	0.707 E20	.5
370	0.24	6	3.96	0.236 E20	.5
359	0.03	6	3.96	0.0295 E20	.5
373	0.395	0.395	3.96	0.389 E20	.5

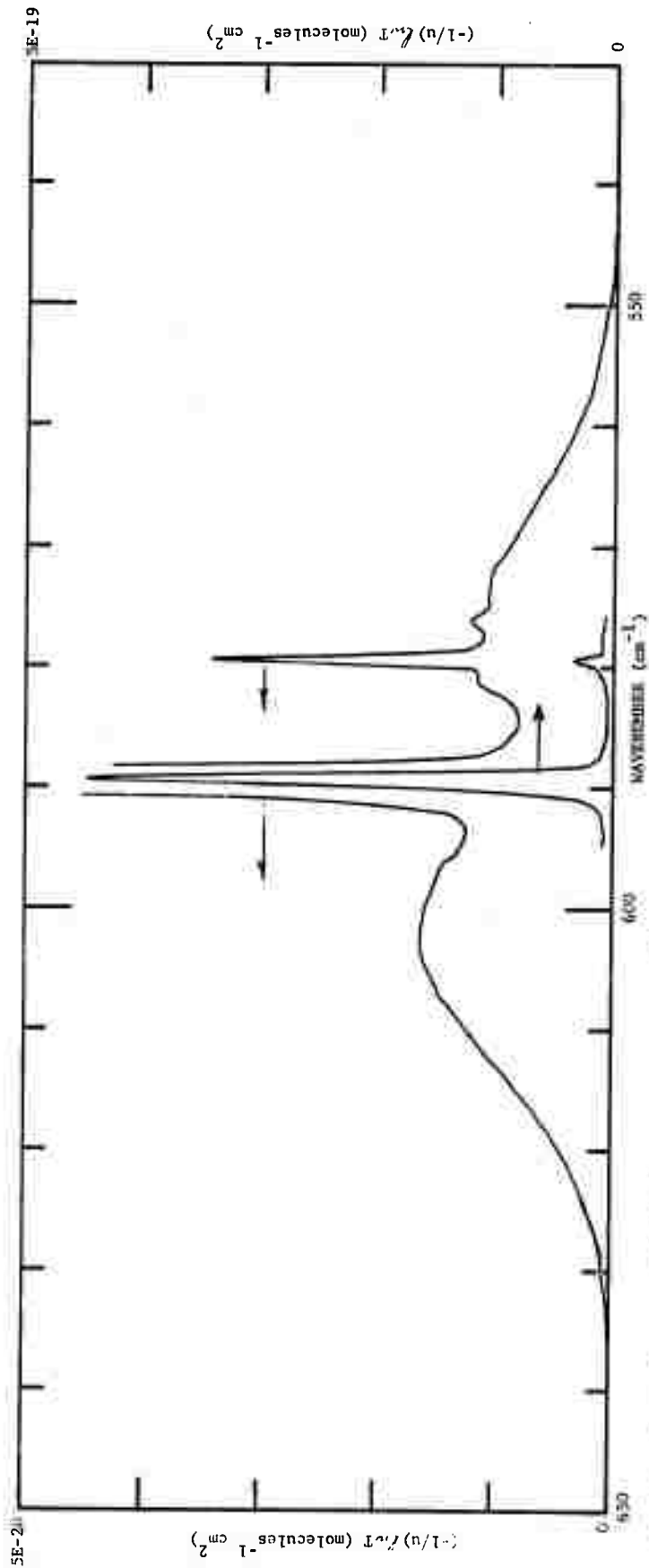


FIG. 4-2. Spectral curves of $(-1/\nu) L_v T$ from 550 to 600 cm^{-1} . The arrows indicate which ordinate unity to use.

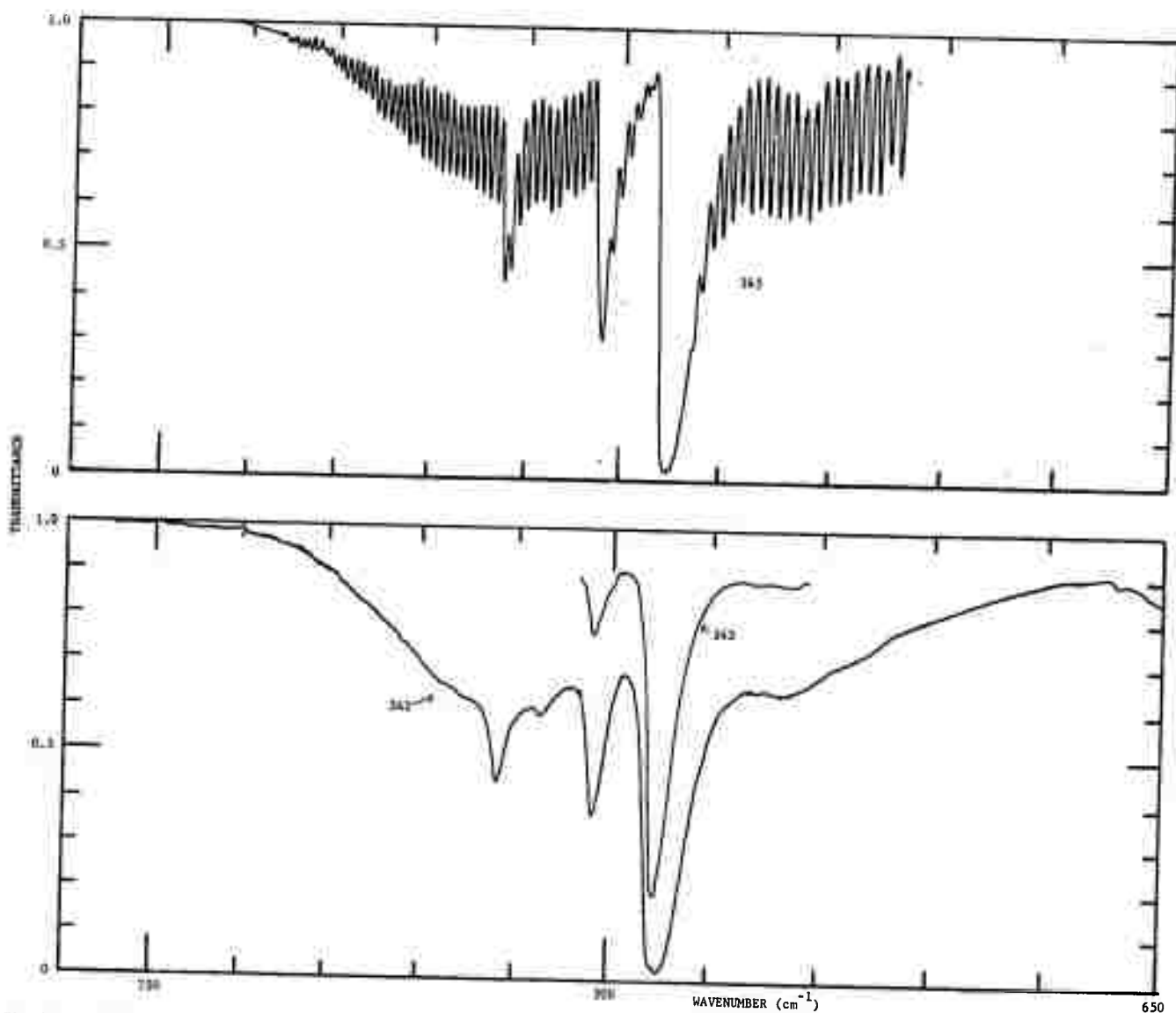


FIG. 4-3. Spectral curves of transmittance from 650 to 755 cm^{-1} for 3 N_2O samples.

Sample No.	p atm	P atm	L cm	u molecules/ cm^2	Slitwidth cm^{-1}
342	1	8	416	103.2 E20	0.56
343	0.263	8	416	27.1 E20	0.56
345	0.335	0.335	1237	101.8 E20	0.38

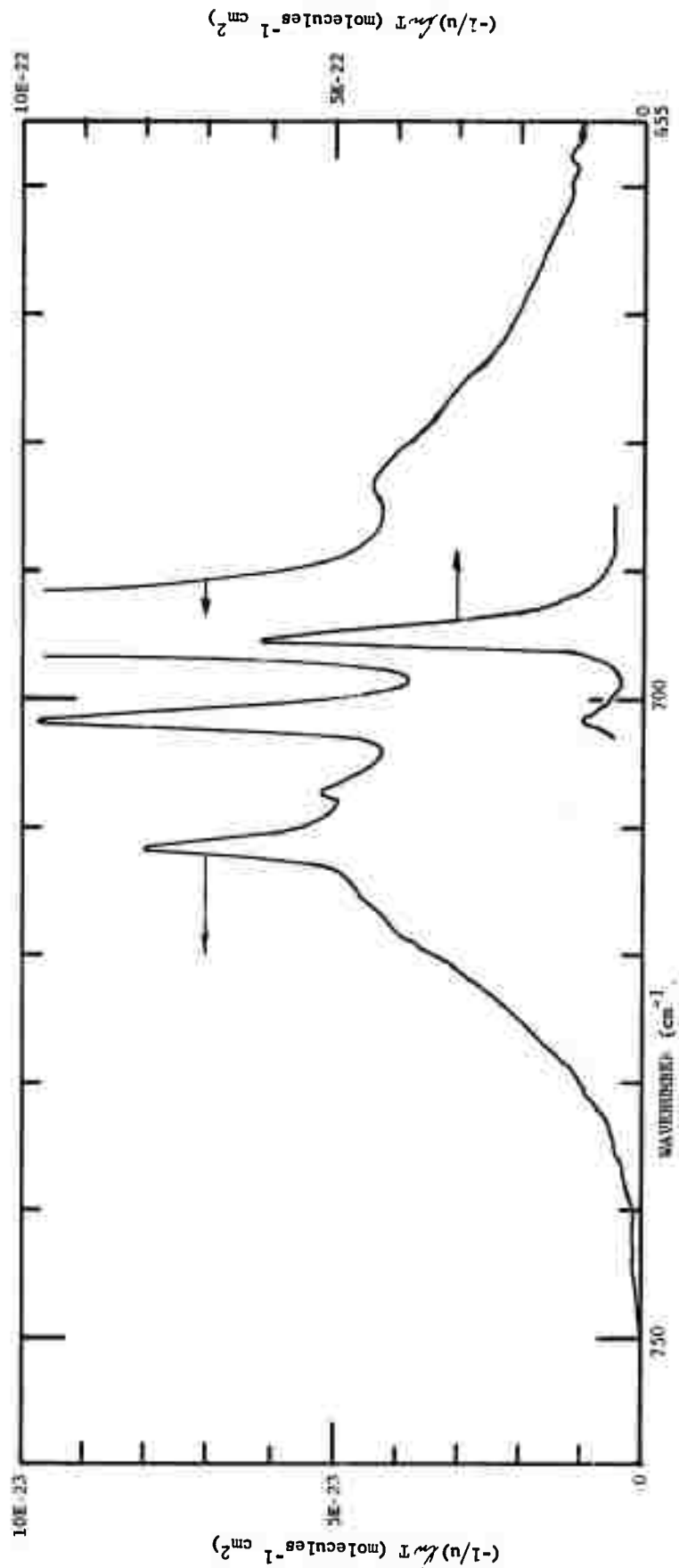


FIG. 4-6. Spectral curves of $(-1/\nu)kT$ from 655 to 755 cm^{-1} . The arrows indicate which ordinate scale to use.

SECTION 5

REFERENCES

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Additional references, that are included for Table 2-1, can be found on page 2-5.

APPENDIX A

ABSTRACTS AND ERRATA FROM FORMER REPORTS

This appendix contains abstracts and errata for all of the reports published on the present contract (No. F19628-69-C-0263, Project No. 5130).

U-4784 "Semi-Annual Technical Report, Investigation of the Absorption of Infrared Radiation by Atmospheric Gases," January 1970.

The continuum absorption by H_2O between 800 and 1250 cm^{-1} and by CO_2 from 780 to 900 cm^{-1} has been measured. The continuum results from the extreme wings of very strong absorption lines centered outside the $800\text{-}1250\text{ cm}^{-1}$ interval. Experimental results are compared with calculated values based on various line shapes. The extreme wings of N_2 -broadened H_2O lines produce less than 0.005 as much continuum absorption as self-broadened H_2O lines at the same pressure. Self-broadened H_2O lines absorb more than Lorentz-shaped lines, but the wings of self-broadened CO_2 lines absorb only approximately 0.01 as much in the $780\text{-}900\text{ cm}^{-1}$ region as if they had the Lorentz shape. The shapes of the wings of the CO_2 lines which produce the continuum between 780 and 900 cm^{-1} are similar to those near 2400 cm^{-1} for both self-broadening and N_2 broadening. Suggestions on methods for using the results for atmospheric transmission calculations are given.

Errata - Figure 3-2, pg 3-4. Ordinate scale should read " C_g ($\text{molecules}^{-1}\text{ cm}^2$)" not C_g^o ($\text{mol}^{-1}\text{ cm}^2\text{ atm}^{-1}$).

U-4829 "Semi-Annual Technical Report, Investigation of the Absorption of Infrared Radiation by Atmospheric Gases," June 1970.

From spectral transmittance curves of very large samples of CO_2 , we have determined coefficients for intrinsic absorption and pressure-induced absorption from approximately 1130 cm^{-1} to 1835 cm^{-1} . Most of the pressure-induced absorption arises from the forbidden ν_1 and $2\nu_2$ bands of the $^{16}\text{C}^{12}\text{O}^{16}$ molecule, and the major portion of the intrinsic absorption arises from the same bands of the $^{16}\text{C}^{12}\text{O}^{18}$ molecule. Curves of the absorption coefficients for samples of CO_2 pressurized to approximately 10 atm, or more, with He are presented throughout most of the region from 1885 cm^{-1} to 2132 cm^{-1} . These curves and a table of the integrated absorption coefficient are adequate to determine the strengths of most of the bands of significance in this region. Spectral transmittance curves of CO_2 absorption between approximately 2065 cm^{-1} and 2100 cm^{-1} are presented for a variety of samples. Curves of the pressure-induced absorption by N_2 are presented for the $2400\text{-}2650 \text{ cm}^{-1}$ region.

Errata - Figure 4-3, pg 4-5. The feature in the curve near 1942 cm^{-1} is probably due to H_2O that appeared as an impurity in the CO_2 sample.

Table 4-1, pg 4-2. The heading for the second column should read " $-1/u \int \ln T(\nu) d\nu$," not " $-1/u \int T(\nu) d\nu$."

U-4897 "Semi-Annual Technical Report, Investigation of the Absorption of Infrared Radiation by Atmospheric Gases: Water, Nitrogen, Nitrous Oxide," January 1971.

The continuum absorption by H_2O between 2400 and 2820 cm^{-1} and by N_2 between 2400 and 2650 cm^{-1} has been measured. The H_2O data cover the temperature range from 338K to 428K and are primarily for pure H_2O . A few preliminary results for $\text{H}_2\text{O} + \text{N}_2$ mixtures are discussed. Calculated values of the continuum-absorption coefficient are compared with the experimental results. From absorption data on samples of pure N_2 and of $\text{N}_2 + \text{O}_2$ at different temperatures, the attenuation by atmospheric N_2 has been calculated for a range of temperatures encountered in the atmosphere. The strengths of several N_2O bands between 1100 and 660 cm^{-1} have been measured and are tabulated.

Errata - Page 3-6 in legend. Lower case p should be upper case P.

$([-\ln T]/p^2L)$ should be $([-\ln T]/P^2L)$.

Page 2-9, line 14. " $25\text{-}50 \text{ cm}^{-1}$ " should be " $250\text{-}500 \text{ cm}^{-1}$."

Page 2-9, the line above Eq. (2-1). Cross out " 1000 cm^{-1} and."

U-4943 "Semi-Annual Technical Report No. 3, Investigation of the Absorption of Infrared Radiation by Nitrous Oxide from 4000 to 6700 cm^{-1} (2.5 to 1.5 μm)," June 1971.

All of the N_2O bands expected to absorb significantly between 4000 and 6700 cm^{-1} have been listed, and the strengths of several of the stronger bands have been determined. Spectral curves are shown for samples at low pressure so that the line structure remains and for samples at approximately 15 atm with the structure smoothed out. The amount of absorption between 6600 and 6650 cm^{-1} on the high wavenumber side of the head of the 00^0_3 band indicates that the extreme wings of the lines absorb less than Lorentz-shaped lines with the same strengths and widths.

U-4995 "Semi-Annual Technical Report, Investigation of the Absorption of Infrared Radiation by Nitrous Oxide from 760 to 2380 cm^{-1} (13.2 to 4.2 μm)," December 1971.

Experimental data are presented on the absorption by a variety of N_2O samples between 760 and 2380 cm^{-1} . Most of the absorption between 760 and 850 cm^{-1} is due to extreme wings of lines centered outside the interval. Strengths of the important band systems are given. Curves of transmittance and tables of integrated absorptance and the integrated absorption coefficient provided detailed information on the absorption. The objective of the study is to provide the data required to determine the parameters of all N_2O absorption lines that absorb significantly over any atmospheric path of interest.

Errata - Page 2-5, second line from bottom. "fpr" should read "for." Document Control Data, last page, title should read "13.2" not "13.1."